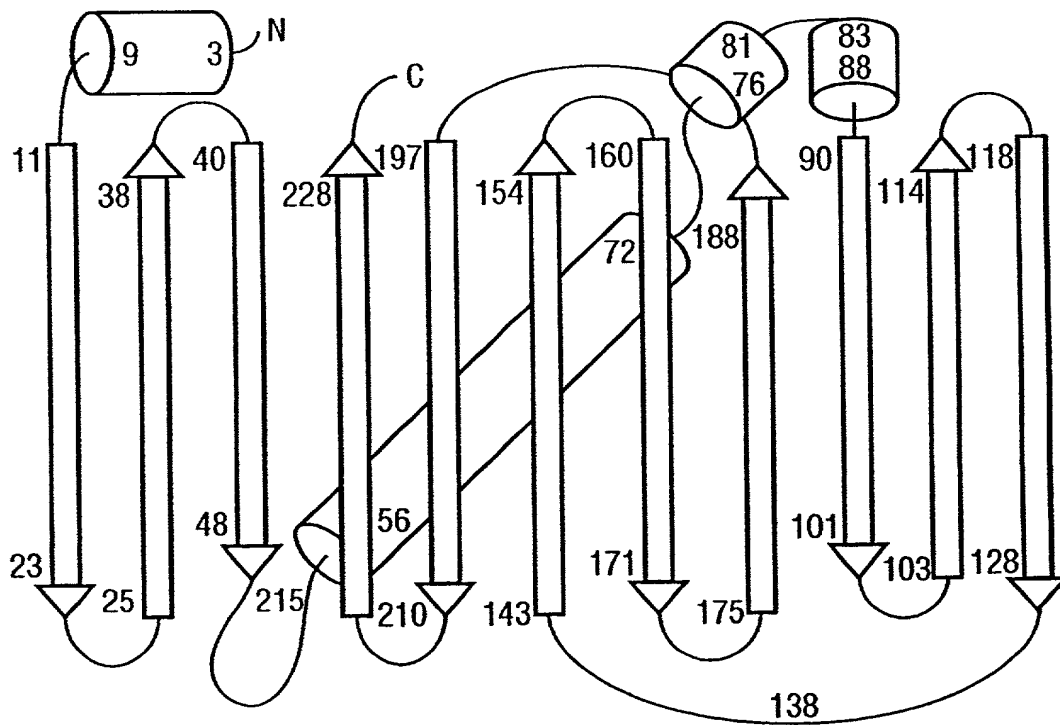
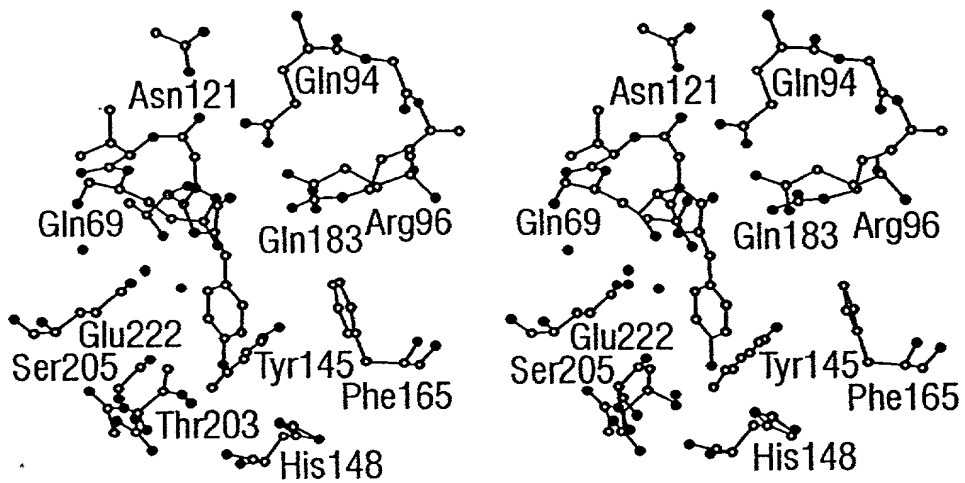


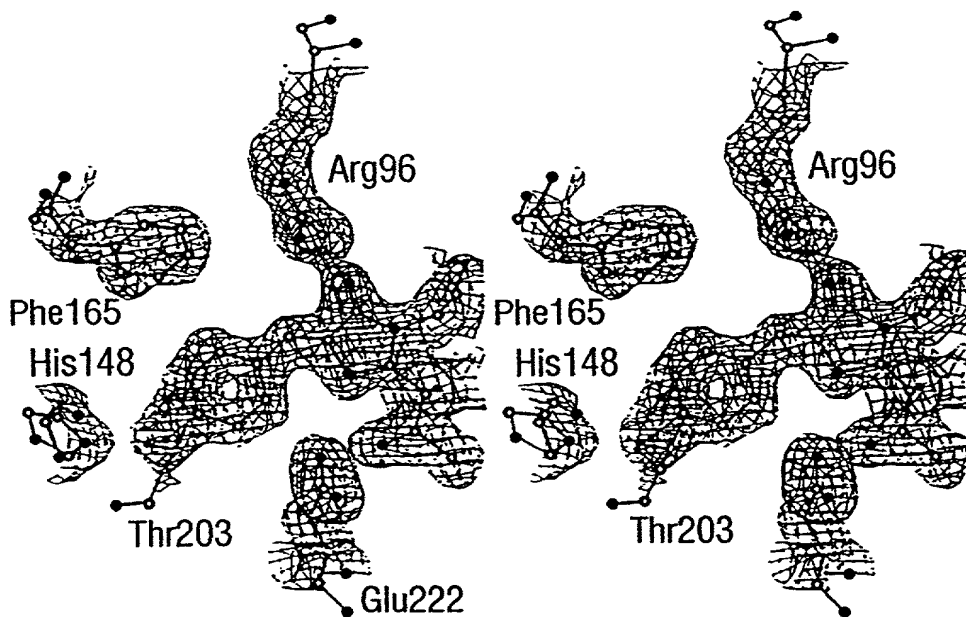
**FIG. 1A**



**FIG. 1B**



**FIG. 2A**



**FIG. 2B**



(xi) SEQUENCE DESCRIPTION:

SEQ ID NO:1:

SEQ ID NO:2:

|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| ATG | AGT | AAA | GGA | GAA | GAA | CTT | TTC | ACT | GGA | GTT | GTC | CCA | ATT | CTT | GTT | 48  |
| Met | Ser | Lys | Gly | Glu | Glu | Leu | Phe | Thr | Gly | Val | Val | Pro | Ile | Leu | Val |     |
| 1   |     |     |     | 5   |     |     |     |     | 10  |     |     |     |     | 15  |     |     |
| GAA | TTA | GAT | GGT | GAT | GTT | AAT | GGG | CAC | AAA | TTT | TCT | GTC | AGT | GGA | GAG | 96  |
| Glu | Leu | Asp | Gly | Asp | Val | Asn | Gly | His | Lys | Phe | Ser | Val | Ser | Gly | Glu |     |
|     |     |     | 20  |     |     |     |     | 25  |     |     |     |     | 30  |     |     |     |
| GGT | GAA | GGT | GAT | GCA | ACA | TAC | GGA | AAA | CTT | ACC | CTT | AAA | TTT | ATT | TGC | 144 |
| Gly | Glu | Gly | Asp | Ala | Thr | Tyr | Gly | Lys | Leu | Thr | Leu | Lys | Phe | Ile | Cys |     |
|     |     |     | 35  |     |     |     | 40  |     |     |     |     | 45  |     |     |     |     |
| ACT | ACT | GGA | AAA | CTA | CCT | GTT | CCA | TGG | CCA | ACA | CTT | GTC | ACT | ACT | TTC | 192 |
| Thr | Thr | Gly | Lys | Leu | Pro | Val | Pro | Trp | Pro | Thr | Leu | Val | Thr | Thr | Phe |     |
|     |     |     | 50  |     |     | 55  |     |     |     |     | 60  |     |     |     |     |     |
| TCT | TAT | GGT | GTT | CAA | TGC | TTT | TCA | AGA | TAC | CCA | GAT | CAT | ATG | AAA | CGG | 240 |
| Ser | Tyr | Gly | Val | Gln | Cys | Phe | Ser | Arg | Tyr | Pro | Asp | His | Met | Lys | Arg |     |
|     |     |     |     | 70  |     |     |     |     |     | 75  |     |     |     | 80  |     |     |
| CAT | GAC | TTT | TTC | AAG | AGT | GCC | ATG | CCC | GAA | GGT | TAT | GTA | CAG | GAA | AGA | 288 |
| His | Asp | Phe | Phe | Lys | Ser | Ala | Met | Pro | Glu | Gly | Tyr | Val | Gln | Glu | Arg |     |
|     |     |     |     | 85  |     |     |     | 90  |     |     |     |     | 95  |     |     |     |
| ACT | ATA | TTT | TTC | AAA | GAT | GAC | GGG | AAC | TAC | AAG | ACA | CGT | GCT | GAA | GTC | 336 |
| Thr | Ile | Phe | Phe | Lys | Asp | Asp | Gly | Asn | Tyr | Lys | Thr | Arg | Ala | Glu | Val |     |
|     |     |     | 100 |     |     |     |     | 105 |     |     |     |     | 110 |     |     |     |
| AAG | TTT | GAA | GGT | GAT | ACC | CTT | GTT | AAT | AGA | ATC | GAG | TTA | AAA | GGT | ATT | 384 |
| Lys | Phe | Glu | Gly | Asp | Thr | Leu | Val | Asn | Arg | Ile | Glu | Leu | Lys | Gly | Ile |     |
|     |     |     | 115 |     |     |     | 120 |     |     |     |     | 125 |     |     |     |     |
| GAT | TTT | AAA | GAA | GAT | GGA | AAC | ATT | CTT | GGA | CAC | AAA | TTG | GAA | TAC | AAC | 432 |
| Asp | Phe | Lys | Glu | Asp | Gly | Asn | Ile | Leu | Gly | His | Lys | Leu | Glu | Tyr | Asn |     |
|     |     |     | 130 |     |     | 135 |     |     |     |     | 140 |     |     |     |     |     |
| TAT | AAC | TCA | CAC | AAT | GTA | TAC | ATC | ATG | GCA | GAC | AAA | CAA | AAG | AAT | GGA | 480 |
| Tyr | Asn | Ser | His | Asn | Val | Tyr | Ile | Met | Ala | Asp | Lys | Gln | Lys | Asn | Gly |     |
|     |     |     |     | 150 |     |     |     |     |     | 155 |     |     |     |     | 160 |     |
| ATC | AAA | GTT | AAC | TTC | AAA | ATT | AGA | CAC | AAC | ATT | GAA | GAT | GGA | AGC | GTT | 528 |
| Ile | Lys | Val | Asn | Phe | Lys | Ile | Arg | His | Asn | Ile | Glu | Asp | Gly | Ser | Val |     |
|     |     |     |     | 165 |     |     |     |     | 170 |     |     |     |     | 175 |     |     |
| CAA | CTA | GCA | GAC | CAT | TAT | CAA | CAA | AAT | ACT | CCA | ATT | GGC | GAT | GGC | CCT | 576 |
| Gln | Leu | Ala | Asp | His | Tyr | Gln | Gln | Asn | Thr | Pro | Ile | Gly | Asp | Gly | Pro |     |
|     |     |     | 180 |     |     |     |     | 185 |     |     |     |     | 190 |     |     |     |
| GTC | CTT | TTA | CCA | GAC | AAC | CAT | TAC | CTG | TCC | ACA | CAA | TCT | GCC | CTT | TCG | 624 |
| Val | Leu | Leu | Pro | Asp | Asn | His | Tyr | Leu | Ser | Thr | Gln | Ser | Ala | Leu | Ser |     |
|     |     |     | 195 |     |     |     | 200 |     |     |     |     | 205 |     |     |     |     |
| AAA | GAT | CCC | AAC | GAA | AAG | AGA | GAC | CAC | ATG | GTC | CTT | CTT | GAG | TTT | GTA | 672 |
| Lys | Asp | Pro | Asn | Glu | Lys | Arg | Asp | His | Met | Val | Leu | Leu | Glu | Phe | Val |     |
|     |     |     | 210 |     |     | 215 |     |     |     |     | 220 |     |     |     |     |     |
| ACA | GCT | GCT | GGG | ATT | ACA | CAT | GGC | ATG | GAT | GAA | CTA | TAC | AAA | TA  |     | 717 |
| Thr | Ala | Ala | Gly | Ile | Thr | His | Gly | Met | Asp | Glu | Leu | Tyr | Lys |     |     |     |
|     |     |     | 225 |     |     | 230 |     |     |     | 235 |     |     |     |     |     |     |

FIG. 3

T203Y, S65G, S72A humanized codon usage, with an additional amino acid  
ater the start met to provide optimal kozak sequence

|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| ATG | GTG | AGC | AAG | GAG | GAG | CTG | TTC | ACC | GGG | GTG | GTG | CCC | ATC | CTG | GTC | GAG |
| Met | Val | Ser | Lys | Gly | Glu | Glu | Leu | Phe | Thr | Gly | Val | Val | Pro | Ile | Leu | Val |
| CTG | GAC | GGC | GAC | GTA | AAC | GGC | CAC | AAG | TTC | AGC | GTG | TCC | GGC | GAG | GGC | GAG |
| Leu | Asp | Gly | Asp | Val | Asn | Gly | His | Lys | Phe | Ser | Val | Ser | Gly | Glu | Gly | Glu |
| GAT | GCC | ACC | TAC | GGC | AAG | CTG | ACC | CTG | AAG | TTC | ATC | TGC | ACC | ACC | GGC | AAG |
| Asp | Ala | Thr | Tyr | Gly | Lys | Leu | Thr | Leu | Lys | Phe | Ile | Cys | Thr | Thr | Gly | Lys |
| CCC | GTG | CCC | TGG | CCC | ACC | CTC | GTG | ACC | ACC | TTC | GGC | TAC | GGC | GTG | CAG | TGC |
| Pro | Val | Pro | Trp | Pro | Thr | Leu | Val | Thr | Thr | Phe | Gly | Tyr | Gly | Val | Gln | Cys |
| GCC | CGC | TAC | CCC | GAC | CAC | ATG | AAG | CAG | CAC | GAC | TTC | TTC | AAG | TCC | GCC | ATG |
| Ala | Arg | Tyr | Pro | Asp | His | Met | Lys | Gln | His | Asp | Phe | Phe | Lys | Ser | Ala | Met |
| GAA | GGC | TAC | GTC | CAG | GAG | CGC | ACC | ATC | TTC | TTC | AAG | GAC | GAC | GGC | AAC | TAC |
| Glu | Gly | Tyr | Val | Gln | Glu | Arg | Thr | Ile | Phe | Phe | Lys | Asp | Asp | Gly | Asn | Tyr |
| ACC | CGC | GCC | GAG | GTG | AAG | TTC | GAG | GGC | GAC | ACC | CTG | GTG | AAC | CGC | ATC | GAG |
| Thr | Arg | Ala | Glu | Val | Lys | Phe | Glu | Gly | Asp | Thr | Leu | Val | Asn | Arg | Ile | Glu |
| AAG | GGC | ATC | GAC | TTC | AAG | GAG | GAC | GGC | AAC | ATC | CTG | GGG | CAC | AAG | CTG | GAG |
| Lys | Gly | Ile | Asp | Phe | Lys | Glu | Asp | Gly | Asn | Ile | Leu | Gly | His | Lys | Leu | Glu |
| AAC | TAC | AAC | AGC | CAC | AAC | GTC | TAT | ATC | ATG | GCC | GAC | AAG | CAG | AAG | AAC | GGC |
| Asn | Tyr | Asn | Ser | His | Asn | Val | Tyr | Ile | Met | Ala | Asp | Lys | Gln | Lys | Asn | Gly |

**FIG. 4A**

|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
|     |     | 495 |     | 504 |     | 513 |     | 522 |     | 531 |     | 540 |     |     |     |     |     |
| AAG | GTG | AAC | TTC | AAG | ATC | CGC | CAC | AAC | ATC | GAG | GAC | GCC | AGC | GTG | CAG | CTC | GCC |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Lys | Val | Asn | Phe | Lys | Ile | Arg | His | Asn | Ile | Glu | Asp | Gly | Ser | Val | Gln | Leu | Ala |
|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|     |     | 549 |     | 558 |     | 567 |     | 576 |     | 585 |     | 594 |     |     |     |     |     |
| GAC | CAC | TAC | CAG | CAG | AAC | ACC | CCC | ATC | GGC | GAC | GGC | CCC | GTG | CTG | CTG | CCC | GAC |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Asp | His | Tyr | Gln | Gln | Asn | Thr | Pro | Ile | Gly | Asp | Gly | Pro | Val | Leu | Leu | Pro | Asp |
|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|     |     | 603 |     | 612 |     | 621 |     | 630 |     | 639 |     | 648 |     |     |     |     |     |
| AAC | CAC | TAC | CTG | AGC | TAC | CAG | TCC | GCC | CTG | AGC | AAA | GAC | CCC | AAC | GAG | AAG | CGC |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Asn | His | Tyr | Leu | Ser | Tyr | Gln | Ser | Ala | Leu | Ser | Lys | Asp | Pro | Asn | Glu | Lys | Arg |
|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|     |     | 657 |     | 666 |     | 675 |     | 684 |     | 693 |     | 702 |     |     |     |     |     |
| GAT | CAC | ATG | GTC | CTG | CTG | GAG | TTC | GTG | ACC | GCC | GCC | GGG | ATC | ACT | CAC | GGC | ATG |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Asp | His | Met | Val | Leu | Leu | Glu | Phe | Val | Thr | Ala | Ala | Gly | Ile | Thr | His | Gly | Met |
|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|     |     | 711 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| GAC | GAG | CTG | TAC | AAG | TAA | 3'  |     |     |     |     |     |     |     |     |     |     |     |
| --- | --- | --- | --- | --- | --- | --- |     |     |     |     |     |     |     |     |     |     |     |
| Asp | Glu | Leu | Tyr | Lys | *** |     |     |     |     |     |     |     |     |     |     |     |     |

**FIG. 4B**

|        |          |          |          |       |        |          |        |             |
|--------|----------|----------|----------|-------|--------|----------|--------|-------------|
| CRYST1 | 51.767   | 62.845   | 70.666   | 90.00 | 90.00  | 90.00    |        |             |
| ORIGX1 | 1.000000 | 0.000000 | 0.000000 |       |        | 0.000000 |        |             |
| ORIGX2 | 0.000000 | 1.000000 | 0.000000 |       |        | 0.000000 |        |             |
| ORIGX3 | 0.000000 | 0.000000 | 1.000000 |       |        | 0.000000 |        |             |
| SCALE1 | 0.019317 | 0.000000 | 0.000000 |       |        | 0.000000 |        |             |
| SCALE2 | 0.000000 | 0.015912 | 0.000000 |       |        | 0.000000 |        |             |
| SCALE3 | 0.000000 | 0.000000 | 0.014151 |       |        | 0.000000 |        |             |
| ATOM   | 1        | N        | SER      | 2     | 28.888 | 9.409    | 52.301 | 1.00 85.05  |
| ATOM   | 2        | CA       | SER      | 2     | 27.638 | 10.125   | 52.516 | 1.00 80.05  |
| ATOM   | 3        | C        | SER      | 2     | 26.499 | 9.639    | 51.644 | 1.00 85.36  |
| ATOM   | 4        | O        | SER      | 2     | 26.606 | 8.656    | 50.915 | 1.00 84.56  |
| ATOM   | 5        | CB       | SER      | 2     | 27.783 | 11.635   | 52.378 | 1.00 70.97  |
| ATOM   | 6        | OG       | SER      | 2     | 27.690 | 12.033   | 51.012 | 1.00 44.08  |
| ATOM   | 7        | N        | LYS      | 3     | 25.418 | 10.403   | 51.731 | 1.00 87.71  |
| ATOM   | 8        | CA       | LYS      | 3     | 24.141 | 10.191   | 51.036 | 1.00 87.15  |
| ATOM   | 9        | C        | LYS      | 3     | 24.214 | 10.266   | 49.497 | 1.00 76.86  |
| ATOM   | 10       | O        | LYS      | 3     | 24.107 | 9.258    | 48.774 | 1.00 78.27  |
| ATOM   | 11       | CB       | LYS      | 3     | 23.127 | 11.240   | 51.521 | 1.00 89.44  |
| ATOM   | 12       | CG       | LYS      | 3     | 21.768 | 10.697   | 51.949 | 1.00 75.06  |
| ATOM   | 13       | CD       | LYS      | 3     | 20.681 | 11.781   | 51.987 | 1.00 76.58  |
| ATOM   | 14       | CE       | LYS      | 3     | 20.711 | 12.655   | 53.243 | 1.00 68.55  |
| ATOM   | 15       | NZ       | LYS      | 3     | 20.816 | 14.103   | 52.953 | 1.00 46.24  |
| ATOM   | 16       | N        | GLY      | 4     | 24.318 | 11.495   | 49.015 | 1.00 53.62  |
| ATOM   | 17       | CA       | GLY      | 4     | 24.297 | 11.798   | 47.605 | 1.00 45.97  |
| ATOM   | 18       | C        | GLY      | 4     | 25.425 | 11.206   | 46.796 | 1.00 31.90  |
| ATOM   | 19       | O        | GLY      | 4     | 25.234 | 10.923   | 45.619 | 1.00 33.63  |
| ATOM   | 20       | N        | GLU      | 5     | 26.606 | 11.082   | 47.420 | 1.00 32.54  |
| ATOM   | 21       | CA       | GLU      | 5     | 27.821 | 10.598   | 46.726 | 1.00 32.57  |
| ATOM   | 22       | C        | GLU      | 5     | 27.523 | 9.590    | 45.616 | 1.00 28.40  |
| ATOM   | 23       | O        | GLU      | 5     | 27.850 | 9.803    | 44.444 | 1.00 26.12  |
| ATOM   | 24       | CB       | GLU      | 5     | 28.873 | 10.053   | 47.718 | 1.00 38.53  |
| ATOM   | 25       | CG       | GLU      | 5     | 30.337 | 10.461   | 47.425 | 1.00 41.36  |
| ATOM   | 26       | CD       | GLU      | 5     | 31.311 | 9.584    | 48.170 | 1.00 90.82  |
| ATOM   | 27       | OE1      | GLU      | 5     | 31.508 | 9.677    | 49.381 | 1.00 74.80  |
| ATOM   | 28       | OE2      | GLU      | 5     | 31.839 | 8.653    | 47.403 | 1.00 100.00 |
| ATOM   | 29       | N        | GLU      | 6     | 26.883 | 8.499    | 46.017 | 1.00 28.57  |
| ATOM   | 30       | CA       | GLU      | 6     | 26.479 | 7.410    | 45.150 | 1.00 31.50  |
| ATOM   | 31       | C        | GLU      | 6     | 25.561 | 7.837    | 43.979 | 1.00 31.10  |
| ATOM   | 32       | O        | GLU      | 6     | 25.479 | 7.142    | 42.955 | 1.00 30.96  |
| ATOM   | 33       | CB       | GLU      | 6     | 25.780 | 6.330    | 45.992 | 1.00 35.64  |
| ATOM   | 34       | CG       | GLU      | 6     | 25.260 | 6.893    | 47.338 | 1.00 55.53  |
| ATOM   | 35       | N        | LEU      | 7     | 24.864 | 8.966    | 44.138 | 1.00 22.26  |

**FIG. 5A**

|      |    |     |     |    |        |        |        |      |       |
|------|----|-----|-----|----|--------|--------|--------|------|-------|
| ATOM | 36 | CA  | LEU | 7  | 23.954 | 9.456  | 43.089 | 1.00 | 21.61 |
| ATOM | 37 | C   | LEU | 7  | 24.693 | 10.061 | 41.917 | 1.00 | 16.90 |
| ATOM | 38 | O   | LEU | 7  | 24.152 | 10.250 | 40.836 | 1.00 | 18.38 |
| ATOM | 39 | CB  | LEU | 7  | 23.050 | 10.548 | 43.665 | 1.00 | 22.41 |
| ATOM | 40 | CG  | LEU | 7  | 21.672 | 10.058 | 44.098 | 1.00 | 32.84 |
| ATOM | 41 | CD1 | LEU | 7  | 21.597 | 8.536  | 44.074 | 1.00 | 31.64 |
| ATOM | 42 | CD2 | LEU | 7  | 21.332 | 10.591 | 45.485 | 1.00 | 33.14 |
| ATOM | 43 | N   | PHE | 8  | 25.944 | 10.407 | 42.157 | 1.00 | 20.75 |
| ATOM | 44 | CA  | PHE | 8  | 26.740 | 11.132 | 41.159 | 1.00 | 21.64 |
| ATOM | 45 | C   | PHE | 8  | 27.818 | 10.333 | 40.427 | 1.00 | 30.59 |
| ATOM | 46 | O   | PHE | 8  | 28.590 | 10.856 | 39.600 | 1.00 | 30.05 |
| ATOM | 47 | CB  | PHE | 8  | 27.309 | 12.376 | 41.820 | 1.00 | 16.95 |
| ATOM | 48 | CG  | PHE | 8  | 26.222 | 13.355 | 42.163 | 1.00 | 13.29 |
| ATOM | 49 | CD1 | PHE | 8  | 25.672 | 13.378 | 43.447 | 1.00 | 17.27 |
| ATOM | 50 | CD2 | PHE | 8  | 25.726 | 14.227 | 41.189 | 1.00 | 13.12 |
| ATOM | 51 | CE1 | PHE | 8  | 24.661 | 14.290 | 43.772 | 1.00 | 15.14 |
| ATOM | 52 | CE2 | PHE | 8  | 24.712 | 15.137 | 41.499 | 1.00 | 13.19 |
| ATOM | 53 | CZ  | PHE | 8  | 24.192 | 15.170 | 42.794 | 1.00 | 5.69  |
| ATOM | 54 | N   | THR | 9  | 27.798 | 9.074  | 40.699 | 1.00 | 27.35 |
| ATOM | 55 | CA  | THR | 9  | 28.704 | 8.122  | 40.175 | 1.00 | 34.93 |
| ATOM | 56 | C   | THR | 9  | 28.709 | 7.998  | 38.636 | 1.00 | 45.22 |
| ATOM | 57 | O   | THR | 9  | 29.642 | 7.452  | 38.062 | 1.00 | 50.55 |
| ATOM | 58 | CB  | THR | 9  | 28.447 | 6.795  | 40.892 | 1.00 | 44.60 |
| ATOM | 59 | OG1 | THR | 9  | 29.629 | 6.330  | 41.527 | 1.00 | 40.40 |
| ATOM | 60 | CG2 | THR | 9  | 27.801 | 5.779  | 39.959 | 1.00 | 29.76 |
| ATOM | 61 | N   | GLY | 10 | 27.690 | 8.510  | 37.956 | 1.00 | 30.53 |
| ATOM | 62 | CA  | GLY | 10 | 27.689 | 8.458  | 36.507 | 1.00 | 23.21 |
| ATOM | 63 | C   | GLY | 10 | 27.144 | 9.746  | 35.914 | 1.00 | 16.55 |
| ATOM | 64 | O   | GLY | 10 | 27.011 | 10.729 | 36.617 | 1.00 | 25.70 |
| ATOM | 65 | N   | VAL | 11 | 26.835 | 9.719  | 34.629 | 1.00 | 16.39 |
| ATOM | 66 | CA  | VAL | 11 | 26.209 | 10.863 | 33.971 | 1.00 | 22.28 |
| ATOM | 67 | C   | VAL | 11 | 24.758 | 11.020 | 34.479 | 1.00 | 29.60 |
| ATOM | 68 | O   | VAL | 11 | 23.972 | 10.062 | 34.456 | 1.00 | 20.43 |
| ATOM | 69 | CB  | VAL | 11 | 26.173 | 10.664 | 32.467 | 1.00 | 30.87 |
| ATOM | 70 | CG1 | VAL | 11 | 25.912 | 11.980 | 31.734 | 1.00 | 31.75 |
| ATOM | 71 | CG2 | VAL | 11 | 27.480 | 10.048 | 32.015 | 1.00 | 33.85 |
| ATOM | 72 | N   | VAL | 12 | 24.417 | 12.227 | 34.931 | 1.00 | 20.12 |
| ATOM | 73 | CA  | VAL | 12 | 23.080 | 12.561 | 35.433 | 1.00 | 12.88 |
| ATOM | 74 | C   | VAL | 12 | 22.407 | 13.624 | 34.516 | 1.00 | 14.37 |
| ATOM | 75 | O   | VAL | 12 | 23.007 | 14.639 | 34.179 | 1.00 | 13.42 |
| ATOM | 76 | CB  | VAL | 12 | 23.270 | 13.077 | 36.839 | 1.00 | 15.01 |

**FIG. 5B**



|      |     |        |    |        |        |        |            |
|------|-----|--------|----|--------|--------|--------|------------|
| ATOM | 77  | CG1VAL | 12 | 22.000 | 13.662 | 37.422 | 1.00 17.57 |
| ATOM | 78  | CG2VAL | 12 | 23.781 | 11.936 | 37.728 | 1.00 16.55 |
| ATOM | 79  | N PRO  | 13 | 21.180 | 13.382 | 34.066 | 1.00 14.72 |
| ATOM | 80  | CA PRO | 13 | 20.493 | 14.382 | 33.265 | 1.00 10.76 |
| ATOM | 81  | C PRO  | 13 | 20.116 | 15.589 | 34.141 | 1.00 7.65  |
| ATOM | 82  | O PRO  | 13 | 19.797 | 15.468 | 35.337 | 1.00 15.14 |
| ATOM | 83  | CB PRO | 13 | 19.225 | 13.707 | 32.745 | 1.00 17.36 |
| ATOM | 84  | CG PRO | 13 | 19.043 | 12.422 | 33.550 | 1.00 19.69 |
| ATOM | 85  | CD PRO | 13 | 20.315 | 12.195 | 34.340 | 1.00 15.41 |
| ATOM | 86  | N ILE  | 14 | 20.196 | 16.766 | 33.557 | 1.00 14.91 |
| ATOM | 87  | CA ILE | 14 | 19.893 | 17.991 | 34.266 | 1.00 12.93 |
| ATOM | 88  | C ILE  | 14 | 18.768 | 18.760 | 33.596 | 1.00 12.08 |
| ATOM | 89  | O ILE  | 14 | 18.724 | 18.878 | 32.399 | 1.00 11.04 |
| ATOM | 90  | CB ILE | 14 | 21.109 | 18.905 | 34.325 | 1.00 16.54 |
| ATOM | 91  | CG1ILE | 14 | 22.271 | 18.169 | 35.015 | 1.00 18.08 |
| ATOM | 92  | CG2ILE | 14 | 20.783 | 20.207 | 35.084 | 1.00 11.56 |
| ATOM | 93  | CD1ILE | 14 | 23.642 | 18.836 | 34.738 | 1.00 16.15 |
| ATOM | 94  | N LEU  | 15 | 17.899 | 19.307 | 34.421 | 1.00 13.85 |
| ATOM | 95  | CA LEU | 15 | 16.811 | 20.136 | 33.955 | 1.00 14.82 |
| ATOM | 96  | C LEU  | 15 | 16.915 | 21.474 | 34.685 | 1.00 3.62  |
| ATOM | 97  | O LEU  | 15 | 17.080 | 21.509 | 35.901 | 1.00 10.00 |
| ATOM | 98  | CB LEU | 15 | 15.462 | 19.450 | 34.285 | 1.00 21.25 |
| ATOM | 99  | CG LEU | 15 | 14.412 | 19.541 | 33.199 | 1.00 40.50 |
| ATOM | 100 | CD1LEU | 15 | 13.279 | 20.440 | 33.679 | 1.00 46.97 |
| ATOM | 101 | CD2LEU | 15 | 15.008 | 20.098 | 31.913 | 1.00 49.22 |
| ATOM | 102 | N VAL  | 16 | 16.885 | 22.556 | 33.919 | 1.00 10.56 |
| ATOM | 103 | CA VAL | 16 | 16.964 | 23.905 | 34.479 | 1.00 10.23 |
| ATOM | 104 | C VAL  | 16 | 15.716 | 24.727 | 34.063 | 1.00 9.47  |
| ATOM | 105 | O VAL  | 16 | 15.347 | 24.748 | 32.904 | 1.00 16.72 |
| ATOM | 106 | CB VAL | 16 | 18.273 | 24.668 | 34.098 | 1.00 12.85 |
| ATOM | 107 | CG1VAL | 16 | 18.226 | 26.075 | 34.691 | 1.00 12.58 |
| ATOM | 108 | CG2VAL | 16 | 19.520 | 23.945 | 34.628 | 1.00 14.24 |
| ATOM | 109 | N GLU  | 17 | 15.059 | 25.317 | 35.060 | 1.00 14.43 |
| ATOM | 110 | CA GLU | 17 | 13.904 | 26.144 | 34.870 | 1.00 13.61 |
| ATOM | 111 | C GLU  | 17 | 14.086 | 27.474 | 35.571 | 1.00 9.38  |
| ATOM | 112 | O GLU  | 17 | 14.331 | 27.524 | 36.765 | 1.00 15.74 |
| ATOM | 113 | CB GLU | 17 | 12.650 | 25.402 | 35.344 | 1.00 14.15 |
| ATOM | 114 | CG GLU | 17 | 12.436 | 24.178 | 34.447 | 1.00 15.37 |
| ATOM | 115 | CD GLU | 17 | 11.865 | 24.573 | 33.105 | 1.00 49.50 |
| ATOM | 116 | OE1GLU | 17 | 11.160 | 25.557 | 32.950 | 1.00 83.46 |
| ATOM | 117 | OE2GLU | 17 | 12.220 | 23.766 | 32.127 | 1.00 38.75 |

**FIG. 5C**

|      |     |     |     |    |        |        |        |      |       |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|
| ATOM | 118 | N   | LEU | 18 | 13.990 | 28.571 | 34.805 | 1.00 | 17.82 |
| ATOM | 119 | CA  | LEU | 18 | 14.116 | 29.914 | 35.401 | 1.00 | 16.61 |
| ATOM | 120 | C   | LEU | 18 | 12.962 | 30.855 | 35.057 | 1.00 | 14.91 |
| ATOM | 121 | O   | LEU | 18 | 12.585 | 30.978 | 33.917 | 1.00 | 14.31 |
| ATOM | 122 | CB  | LEU | 18 | 15.426 | 30.630 | 35.005 | 1.00 | 13.56 |
| ATOM | 123 | CG  | LEU | 18 | 15.533 | 32.049 | 35.579 | 1.00 | 19.27 |
| ATOM | 124 | CD1 | LEU | 18 | 16.740 | 32.182 | 36.489 | 1.00 | 21.40 |
| ATOM | 125 | CD2 | LEU | 18 | 15.682 | 33.033 | 34.438 | 1.00 | 18.38 |
| ATOM | 126 | N   | ASP | 19 | 12.480 | 31.551 | 36.082 | 1.00 | 17.88 |
| ATOM | 127 | CA  | ASP | 19 | 11.476 | 32.577 | 35.940 | 1.00 | 19.57 |
| ATOM | 128 | C   | ASP | 19 | 12.098 | 33.896 | 36.360 | 1.00 | 11.65 |
| ATOM | 129 | O   | ASP | 19 | 12.486 | 34.044 | 37.493 | 1.00 | 16.82 |
| ATOM | 130 | CB  | ASP | 19 | 10.234 | 32.305 | 36.847 | 1.00 | 24.92 |
| ATOM | 131 | CG  | ASP | 19 | 9.305  | 31.262 | 36.282 | 1.00 | 38.46 |
| ATOM | 132 | OD1 | ASP | 19 | 8.572  | 30.587 | 36.989 | 1.00 | 61.49 |
| ATOM | 133 | OD2 | ASP | 19 | 9.337  | 31.189 | 34.949 | 1.00 | 22.44 |
| ATOM | 134 | N   | GLY | 20 | 12.178 | 34.863 | 35.471 | 1.00 | 16.82 |
| ATOM | 135 | CA  | GLY | 20 | 12.784 | 36.101 | 35.908 | 1.00 | 19.52 |
| ATOM | 136 | C   | GLY | 20 | 12.048 | 37.385 | 35.538 | 1.00 | 19.35 |
| ATOM | 137 | O   | GLY | 20 | 11.240 | 37.443 | 34.628 | 1.00 | 18.22 |
| ATOM | 138 | N   | ASP | 21 | 12.401 | 38.407 | 36.286 | 1.00 | 13.19 |
| ATOM | 139 | CA  | ASP | 21 | 11.908 | 39.737 | 36.112 | 1.00 | 16.36 |
| ATOM | 140 | C   | ASP | 21 | 13.039 | 40.683 | 36.424 | 1.00 | 12.77 |
| ATOM | 141 | O   | ASP | 21 | 13.517 | 40.742 | 37.569 | 1.00 | 15.18 |
| ATOM | 142 | CB  | ASP | 21 | 10.701 | 40.036 | 37.040 | 1.00 | 22.26 |
| ATOM | 143 | CG  | ASP | 21 | 10.230 | 41.491 | 37.022 | 1.00 | 30.80 |
| ATOM | 144 | OD1 | ASP | 21 | 10.878 | 42.407 | 36.557 | 1.00 | 27.40 |
| ATOM | 145 | OD2 | ASP | 21 | 9.062  | 41.658 | 37.604 | 1.00 | 45.92 |
| ATOM | 146 | N   | VAL | 22 | 13.464 | 41.393 | 35.397 | 1.00 | 19.66 |
| ATOM | 147 | CA  | VAL | 22 | 14.524 | 42.388 | 35.542 | 1.00 | 25.10 |
| ATOM | 148 | C   | VAL | 22 | 14.010 | 43.780 | 35.154 | 1.00 | 18.26 |
| ATOM | 149 | O   | VAL | 22 | 13.769 | 44.062 | 33.955 | 1.00 | 15.10 |
| ATOM | 150 | CB  | VAL | 22 | 15.803 | 42.012 | 34.750 | 1.00 | 26.57 |
| ATOM | 151 | CG1 | VAL | 22 | 16.861 | 43.127 | 34.896 | 1.00 | 24.27 |
| ATOM | 152 | CG2 | VAL | 22 | 16.365 | 40.710 | 35.297 | 1.00 | 22.98 |
| ATOM | 153 | N   | ASN | 23 | 13.823 | 44.641 | 36.166 | 1.00 | 25.32 |
| ATOM | 154 | CA  | ASN | 23 | 13.319 | 45.993 | 35.908 | 1.00 | 32.81 |
| ATOM | 155 | C   | ASN | 23 | 11.987 | 45.958 | 35.142 | 1.00 | 32.77 |
| ATOM | 156 | O   | ASN | 23 | 11.774 | 46.730 | 34.187 | 1.00 | 30.47 |
| ATOM | 157 | CB  | ASN | 23 | 14.344 | 46.831 | 35.096 | 1.00 | 31.26 |
| ATOM | 158 | CG  | ASN | 23 | 15.374 | 47.607 | 35.938 | 1.00 | 24.72 |

**FIG. 5D**

|      |     |        |    |        |        |        |      |       |
|------|-----|--------|----|--------|--------|--------|------|-------|
| ATOM | 159 | OD1ASN | 23 | 15.795 | 47.183 | 37.024 | 1.00 | 27.22 |
| ATOM | 160 | ND2ASN | 23 | 15.829 | 48.723 | 35.389 | 1.00 | 41.15 |
| ATOM | 161 | N GLY  | 24 | 11.118 | 45.024 | 35.519 | 1.00 | 24.95 |
| ATOM | 162 | CA GLY | 24 | 9.831  | 44.919 | 34.848 | 1.00 | 23.22 |
| ATOM | 163 | C GLY  | 24 | 9.832  | 44.111 | 33.573 | 1.00 | 23.31 |
| ATOM | 164 | O GLY  | 24 | 8.780  | 43.868 | 33.024 | 1.00 | 28.37 |
| ATOM | 165 | N HIS  | 25 | 11.000 | 43.691 | 33.071 | 1.00 | 20.89 |
| ATOM | 166 | CA HIS | 25 | 11.042 | 42.840 | 31.877 | 1.00 | 19.30 |
| ATOM | 167 | C HIS  | 25 | 10.981 | 41.373 | 32.316 | 1.00 | 27.26 |
| ATOM | 168 | O HIS  | 25 | 11.898 | 40.850 | 32.951 | 1.00 | 26.47 |
| ATOM | 169 | CB HIS | 25 | 12.268 | 43.060 | 30.958 | 1.00 | 24.20 |
| ATOM | 170 | CG HIS | 25 | 12.313 | 44.382 | 30.218 | 1.00 | 33.04 |
| ATOM | 171 | ND1HIS | 25 | 12.917 | 45.514 | 30.758 | 1.00 | 37.58 |
| ATOM | 172 | CD2HIS | 25 | 11.876 | 44.716 | 28.971 | 1.00 | 42.76 |
| ATOM | 173 | CE1HIS | 25 | 12.801 | 46.497 | 29.867 | 1.00 | 39.14 |
| ATOM | 174 | NE2HIS | 25 | 12.185 | 46.050 | 28.778 | 1.00 | 42.80 |
| ATOM | 175 | N LYS  | 26 | 9.872  | 40.728 | 32.028 | 1.00 | 25.90 |
| ATOM | 176 | CA LYS | 26 | 9.675  | 39.355 | 32.446 | 1.00 | 26.27 |
| ATOM | 177 | C LYS  | 26 | 10.154 | 38.361 | 31.429 | 1.00 | 27.09 |
| ATOM | 178 | O LYS  | 26 | 10.027 | 38.576 | 30.232 | 1.00 | 25.75 |
| ATOM | 179 | CB LYS | 26 | 8.230  | 39.069 | 32.863 | 1.00 | 27.58 |
| ATOM | 180 | CG LYS | 26 | 7.873  | 39.770 | 34.166 | 1.00 | 44.94 |
| ATOM | 181 | CD LYS | 26 | 6.369  | 39.914 | 34.400 | 1.00 | 71.44 |
| ATOM | 182 | CE LYS | 26 | 6.008  | 41.000 | 35.421 | 1.00 | 45.29 |
| ATOM | 183 | N PHE  | 27 | 10.703 | 37.250 | 31.910 | 1.00 | 22.04 |
| ATOM | 184 | CA PHE | 27 | 11.164 | 36.236 | 30.978 | 1.00 | 18.78 |
| ATOM | 185 | C PHE  | 27 | 11.273 | 34.863 | 31.619 | 1.00 | 14.75 |
| ATOM | 186 | O PHE  | 27 | 11.293 | 34.722 | 32.842 | 1.00 | 15.94 |
| ATOM | 187 | CB PHE | 27 | 12.495 | 36.638 | 30.287 | 1.00 | 21.58 |
| ATOM | 188 | CG PHE | 27 | 13.599 | 36.826 | 31.311 | 1.00 | 22.06 |
| ATOM | 189 | CD1PHE | 27 | 14.490 | 35.791 | 31.612 | 1.00 | 23.61 |
| ATOM | 190 | CD2PHE | 27 | 13.722 | 38.029 | 32.005 | 1.00 | 17.55 |
| ATOM | 191 | CE1PHE | 27 | 15.487 | 35.963 | 32.579 | 1.00 | 16.61 |
| ATOM | 192 | CE2PHE | 27 | 14.747 | 38.234 | 32.931 | 1.00 | 19.75 |
| ATOM | 193 | CZ PHE | 27 | 15.621 | 37.187 | 33.234 | 1.00 | 13.83 |
| ATOM | 194 | N SER  | 28 | 11.370 | 33.857 | 30.752 | 1.00 | 12.40 |
| ATOM | 195 | CA SER | 28 | 11.492 | 32.479 | 31.186 | 1.00 | 15.59 |
| ATOM | 196 | C SER  | 28 | 12.579 | 31.749 | 30.379 | 1.00 | 15.96 |
| ATOM | 197 | O SER  | 28 | 12.699 | 31.933 | 29.167 | 1.00 | 18.99 |
| ATOM | 198 | CB SER | 28 | 10.143 | 31.702 | 31.086 | 1.00 | 14.48 |
| ATOM | 199 | OG SER | 28 | 9.510  | 31.678 | 32.353 | 1.00 | 31.95 |

**FIG. 5E**

|      |     |     |     |    |        |        |        |      |       |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|
| ATOM | 200 | N   | VAL | 29 | 13.335 | 30.902 | 31.073 | 1.00 | 16.73 |
| ATOM | 201 | CA  | VAL | 29 | 14.361 | 30.093 | 30.435 | 1.00 | 14.06 |
| ATOM | 202 | C   | VAL | 29 | 14.258 | 28.614 | 30.187 | 1.00 | 6.80  |
| ATOM | 203 | O   | VAL | 29 | 14.058 | 28.266 | 31.987 | 1.00 | 10.85 |
| ATOM | 204 | CB  | VAL | 29 | 15.768 | 30.570 | 30.839 | 1.00 | 17.96 |
| ATOM | 205 | CG1 | VAL | 29 | 16.826 | 29.599 | 30.234 | 1.00 | 15.30 |
| ATOM | 206 | CG2 | VAL | 29 | 15.989 | 32.001 | 30.357 | 1.00 | 16.37 |
| ATOM | 207 | N   | SER | 30 | 14.462 | 27.781 | 29.824 | 1.00 | 11.31 |
| ATOM | 208 | CA  | SER | 30 | 14.535 | 26.351 | 30.011 | 1.00 | 17.96 |
| ATOM | 209 | C   | SER | 30 | 15.917 | 25.818 | 29.571 | 1.00 | 11.26 |
| ATOM | 210 | O   | SER | 30 | 16.398 | 26.157 | 28.513 | 1.00 | 13.17 |
| ATOM | 211 | CB  | SER | 30 | 13.471 | 25.603 | 29.202 | 1.00 | 19.91 |
| ATOM | 212 | OG  | SER | 30 | 12.249 | 25.667 | 29.882 | 1.00 | 48.74 |
| ATOM | 213 | N   | GLY | 31 | 16.480 | 24.926 | 30.364 | 1.00 | 9.88  |
| ATOM | 214 | CA  | GLY | 31 | 17.718 | 24.321 | 29.977 | 1.00 | 12.44 |
| ATOM | 215 | C   | GLY | 31 | 17.737 | 22.816 | 30.249 | 1.00 | 13.16 |
| ATOM | 216 | O   | GLY | 31 | 17.149 | 22.324 | 31.176 | 1.00 | 12.41 |
| ATOM | 217 | N   | GLU | 32 | 18.459 | 22.112 | 29.433 | 1.00 | 13.44 |
| ATOM | 218 | CA  | GLU | 32 | 18.622 | 20.670 | 29.570 | 1.00 | 13.73 |
| ATOM | 219 | C   | GLU | 32 | 20.079 | 20.297 | 29.262 | 1.00 | 17.33 |
| ATOM | 220 | O   | GLU | 32 | 20.734 | 20.946 | 28.456 | 1.00 | 15.56 |
| ATOM | 221 | CB  | GLU | 32 | 17.761 | 19.893 | 28.543 | 1.00 | 12.67 |
| ATOM | 222 | CG  | GLU | 32 | 16.264 | 20.187 | 28.618 | 1.00 | 26.43 |
| ATOM | 223 | CD  | GLU | 32 | 15.501 | 19.547 | 27.468 | 1.00 | 21.13 |
| ATOM | 224 | OE1 | GLU | 32 | 15.996 | 18.767 | 26.698 | 1.00 | 23.45 |
| ATOM | 225 | OE2 | GLU | 32 | 14.292 | 20.022 | 27.337 | 1.00 | 30.63 |
| ATOM | 226 | N   | GLY | 33 | 20.534 | 19.207 | 29.822 | 1.00 | 15.36 |
| ATOM | 227 | CA  | GLY | 33 | 21.860 | 18.687 | 29.518 | 1.00 | 12.84 |
| ATOM | 228 | C   | GLY | 33 | 22.236 | 17.602 | 30.467 | 1.00 | 14.69 |
| ATOM | 229 | O   | GLY | 33 | 21.390 | 16.919 | 31.011 | 1.00 | 13.56 |
| ATOM | 230 | N   | GLU | 34 | 23.525 | 17.453 | 30.702 | 1.00 | 15.15 |
| ATOM | 231 | CA  | GLU | 34 | 23.971 | 16.450 | 31.621 | 1.00 | 18.14 |
| ATOM | 232 | C   | GLU | 34 | 25.220 | 16.874 | 32.367 | 1.00 | 16.26 |
| ATOM | 233 | O   | GLU | 34 | 25.926 | 17.760 | 31.944 | 1.00 | 18.67 |
| ATOM | 234 | CB  | GLU | 34 | 24.180 | 15.114 | 30.927 | 1.00 | 22.53 |
| ATOM | 235 | CG  | GLU | 34 | 24.948 | 15.261 | 29.624 | 1.00 | 33.78 |
| ATOM | 236 | CD  | GLU | 34 | 24.879 | 14.020 | 28.796 | 1.00 | 55.15 |
| ATOM | 237 | OE1 | GLU | 34 | 25.861 | 13.352 | 28.534 | 1.00 | 45.39 |
| ATOM | 238 | OE2 | GLU | 34 | 23.653 | 13.719 | 28.430 | 1.00 | 56.26 |
| ATOM | 239 | N   | GLY | 35 | 25.461 | 16.222 | 33.485 | 1.00 | 11.20 |
| ATOM | 240 | CA  | GLY | 35 | 26.611 | 16.502 | 34.315 | 1.00 | 10.62 |

**FIG. 5F**

|      |     |     |     |    |        |        |        |      |       |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|
| ATOM | 241 | C   | GLY | 35 | 27.293 | 15.192 | 34.662 | 1.00 | 19.92 |
| ATOM | 242 | O   | GLY | 35 | 26.650 | 14.161 | 34.750 | 1.00 | 16.69 |
| ATOM | 243 | N   | ASP | 36 | 28.594 | 15.238 | 34.860 | 1.00 | 16.92 |
| ATOM | 244 | CA  | ASP | 36 | 29.367 | 14.061 | 35.221 | 1.00 | 16.19 |
| ATOM | 245 | C   | ASP | 36 | 30.396 | 14.505 | 36.233 | 1.00 | 13.94 |
| ATOM | 246 | O   | ASP | 36 | 31.469 | 15.004 | 35.879 | 1.00 | 15.77 |
| ATOM | 247 | CB  | ASP | 36 | 30.032 | 13.457 | 33.948 | 1.00 | 19.98 |
| ATOM | 248 | CG  | ASP | 36 | 30.681 | 12.066 | 34.075 | 1.00 | 31.92 |
| ATOM | 249 | OD1 | ASP | 36 | 31.236 | 11.519 | 33.141 | 1.00 | 30.97 |
| ATOM | 250 | OD2 | ASP | 36 | 30.587 | 11.515 | 35.248 | 1.00 | 25.32 |
| ATOM | 251 | N   | ALA | 37 | 30.015 | 14.402 | 37.490 | 1.00 | 13.40 |
| ATOM | 252 | CA  | ALA | 37 | 30.818 | 14.846 | 38.582 | 1.00 | 12.98 |
| ATOM | 253 | C   | ALA | 37 | 32.181 | 14.145 | 38.637 | 1.00 | 21.94 |
| ATOM | 254 | O   | ALA | 37 | 33.084 | 14.604 | 39.331 | 1.00 | 13.61 |
| ATOM | 255 | CB  | ALA | 37 | 30.070 | 14.741 | 39.916 | 1.00 | 11.49 |
| ATOM | 256 | N   | THR | 38 | 32.307 | 13.016 | 37.945 | 1.00 | 15.63 |
| ATOM | 257 | CA  | THR | 38 | 33.581 | 12.280 | 37.943 | 1.00 | 19.94 |
| ATOM | 258 | C   | THR | 38 | 34.705 | 13.114 | 37.335 | 1.00 | 25.61 |
| ATOM | 259 | O   | THR | 38 | 35.850 | 13.069 | 37.775 | 1.00 | 17.89 |
| ATOM | 260 | CB  | THR | 38 | 33.462 | 10.898 | 37.299 | 1.00 | 22.57 |
| ATOM | 261 | OG1 | THR | 38 | 32.543 | 10.146 | 38.067 | 1.00 | 29.86 |
| ATOM | 262 | CG2 | THR | 38 | 34.821 | 10.213 | 37.355 | 1.00 | 22.90 |
| ATOM | 263 | N   | TYR | 39 | 34.323 | 13.920 | 36.347 | 1.00 | 18.45 |
| ATOM | 264 | CA  | TYR | 39 | 35.210 | 14.837 | 35.675 | 1.00 | 9.39  |
| ATOM | 265 | C   | TYR | 39 | 34.874 | 16.291 | 35.991 | 1.00 | 14.41 |
| ATOM | 266 | O   | TYR | 39 | 35.454 | 17.177 | 35.410 | 1.00 | 16.24 |
| ATOM | 267 | CB  | TYR | 39 | 35.156 | 14.582 | 34.180 | 1.00 | 11.82 |
| ATOM | 268 | CG  | TYR | 39 | 35.426 | 13.137 | 33.929 | 1.00 | 28.73 |
| ATOM | 269 | CD1 | TYR | 39 | 36.715 | 12.633 | 34.065 | 1.00 | 33.75 |
| ATOM | 270 | CD2 | TYR | 39 | 34.392 | 12.249 | 33.642 | 1.00 | 39.19 |
| ATOM | 271 | CE1 | TYR | 39 | 36.982 | 11.276 | 33.828 | 1.00 | 29.75 |
| ATOM | 272 | CE2 | TYR | 39 | 34.635 | 10.885 | 33.435 | 1.00 | 45.41 |
| ATOM | 273 | CZ  | TYR | 39 | 35.943 | 10.410 | 33.570 | 1.00 | 57.62 |
| ATOM | 274 | OH  | TYR | 39 | 36.199 | 9.070  | 33.364 | 1.00 | 70.77 |
| ATOM | 275 | N   | GLY | 40 | 33.935 | 16.525 | 36.929 | 1.00 | 9.94  |
| ATOM | 276 | CA  | GLY | 40 | 33.474 | 17.879 | 37.266 | 1.00 | 7.02  |
| ATOM | 277 | C   | GLY | 40 | 32.952 | 18.600 | 36.004 | 1.00 | 9.45  |
| ATOM | 278 | O   | GLY | 40 | 33.068 | 19.830 | 35.829 | 1.00 | 12.63 |
| ATOM | 279 | N   | LYS | 41 | 32.380 | 17.823 | 35.092 | 1.00 | 5.44  |
| ATOM | 280 | CA  | LYS | 41 | 31.954 | 18.335 | 33.842 | 1.00 | 6.63  |
| ATOM | 281 | C   | LYS | 41 | 30.414 | 18.554 | 33.703 | 1.00 | 20.92 |

**FIG. 5G**

|      |     |     |     |    |        |        |        |      |       |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|
| ATOM | 282 | O   | LYS | 41 | 29.617 | 17.693 | 34.085 | 1.00 | 12.94 |
| ATOM | 283 | CB  | LYS | 41 | 32.360 | 17.357 | 32.827 | 1.00 | 8.27  |
| ATOM | 284 | CG  | LYS | 41 | 32.099 | 17.771 | 31.419 | 1.00 | 13.19 |
| ATOM | 285 | CD  | LYS | 41 | 32.521 | 16.644 | 30.481 | 1.00 | 20.20 |
| ATOM | 286 | CE  | LYS | 41 | 32.690 | 17.068 | 29.032 | 1.00 | 35.79 |
| ATOM | 287 | NZ  | LYS | 41 | 33.113 | 15.954 | 28.147 | 1.00 | 47.56 |
| ATOM | 288 | N   | LEU | 42 | 30.049 | 19.684 | 33.069 | 1.00 | 18.31 |
| ATOM | 289 | CA  | LEU | 42 | 28.643 | 20.064 | 32.794 | 1.00 | 16.08 |
| ATOM | 290 | C   | LEU | 42 | 28.456 | 20.422 | 31.330 | 1.00 | 14.23 |
| ATOM | 291 | O   | LEU | 42 | 29.240 | 21.168 | 30.787 | 1.00 | 14.79 |
| ATOM | 292 | CB  | LEU | 42 | 28.223 | 21.300 | 33.621 | 1.00 | 13.22 |
| ATOM | 293 | CG  | LEU | 42 | 28.007 | 21.061 | 35.082 | 1.00 | 16.70 |
| ATOM | 294 | CD1 | LEU | 42 | 27.894 | 22.406 | 35.782 | 1.00 | 13.79 |
| ATOM | 295 | CD2 | LEU | 42 | 26.732 | 20.243 | 35.295 | 1.00 | 18.70 |
| ATOM | 296 | N   | THR | 43 | 27.395 | 19.914 | 30.672 | 1.00 | 8.04  |
| ATOM | 297 | CA  | THR | 43 | 27.103 | 20.275 | 29.282 | 1.00 | 4.87  |
| ATOM | 298 | C   | THR | 43 | 25.636 | 20.666 | 29.186 | 1.00 | 17.23 |
| ATOM | 299 | O   | THR | 43 | 24.811 | 19.818 | 29.442 | 1.00 | 14.38 |
| ATOM | 300 | CB  | THR | 43 | 27.351 | 19.140 | 28.317 | 1.00 | 21.59 |
| ATOM | 301 | OG1 | THR | 43 | 28.692 | 18.743 | 28.415 | 1.00 | 42.74 |
| ATOM | 302 | CG2 | THR | 43 | 27.073 | 19.675 | 26.917 | 1.00 | 31.23 |
| ATOM | 303 | N   | LEU | 44 | 25.327 | 21.934 | 28.830 | 1.00 | 11.83 |
| ATOM | 304 | CA  | LEU | 44 | 23.944 | 22.409 | 28.847 | 1.00 | 13.81 |
| ATOM | 305 | C   | LEU | 44 | 23.589 | 23.307 | 27.668 | 1.00 | 18.19 |
| ATOM | 306 | O   | LEU | 44 | 24.416 | 23.989 | 27.107 | 1.00 | 13.86 |
| ATOM | 307 | CB  | LEU | 44 | 23.725 | 23.275 | 30.125 | 1.00 | 15.37 |
| ATOM | 308 | CG  | LEU | 44 | 23.369 | 22.584 | 31.456 | 1.00 | 24.69 |
| ATOM | 309 | CD1 | LEU | 44 | 21.869 | 22.381 | 31.601 | 1.00 | 23.20 |
| ATOM | 310 | CD2 | LEU | 44 | 24.083 | 21.286 | 31.650 | 1.00 | 46.18 |
| ATOM | 311 | N   | LYS | 45 | 22.294 | 23.331 | 27.339 | 1.00 | 10.29 |
| ATOM | 312 | CA  | LYS | 45 | 21.752 | 24.224 | 26.358 | 1.00 | 11.94 |
| ATOM | 313 | C   | LYS | 45 | 20.534 | 24.913 | 26.957 | 1.00 | 19.35 |
| ATOM | 314 | O   | LYS | 45 | 19.665 | 24.248 | 27.530 | 1.00 | 18.43 |
| ATOM | 315 | CB  | LYS | 45 | 21.409 | 23.560 | 25.060 | 1.00 | 13.75 |
| ATOM | 316 | CG  | LYS | 45 | 20.878 | 24.556 | 24.045 | 1.00 | 8.83  |
| ATOM | 317 | CD  | LYS | 45 | 20.486 | 23.863 | 22.746 | 1.00 | 26.87 |
| ATOM | 318 | CE  | LYS | 45 | 19.574 | 24.688 | 21.842 | 1.00 | 16.58 |
| ATOM | 319 | NZ  | LYS | 45 | 19.318 | 24.024 | 20.555 | 1.00 | 18.33 |
| ATOM | 320 | N   | PHE | 46 | 20.535 | 26.236 | 26.910 | 1.00 | 12.34 |
| ATOM | 321 | CA  | PHE | 46 | 19.463 | 27.048 | 27.451 | 1.00 | 13.32 |
| ATOM | 322 | C   | PHE | 46 | 18.759 | 27.718 | 26.343 | 1.00 | 18.26 |

**FIG. 5H**



|      |     |     |     |    |        |        |        |      |       |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|
| ATOM | 364 | CA  | LYS | 52 | 14.416 | 37.460 | 23.416 | 1.00 | 35.75 |
| ATOM | 365 | C   | LYS | 52 | 14.827 | 37.726 | 24.861 | 1.00 | 29.65 |
| ATOM | 366 | O   | LYS | 52 | 14.140 | 38.420 | 25.620 | 1.00 | 25.70 |
| ATOM | 367 | CB  | LYS | 52 | 14.577 | 38.714 | 22.582 | 1.00 | 43.37 |
| ATOM | 368 | CG  | LYS | 52 | 15.772 | 38.649 | 21.644 | 1.00 | 78.17 |
| ATOM | 369 | N   | LEU | 53 | 15.983 | 37.190 | 25.250 | 1.00 | 19.22 |
| ATOM | 370 | CA  | LEU | 53 | 16.439 | 37.430 | 26.596 | 1.00 | 13.52 |
| ATOM | 371 | C   | LEU | 53 | 16.717 | 38.932 | 26.775 | 1.00 | 17.76 |
| ATOM | 372 | O   | LEU | 53 | 17.392 | 39.539 | 25.973 | 1.00 | 21.59 |
| ATOM | 373 | CB  | LEU | 53 | 17.705 | 36.567 | 26.845 | 1.00 | 17.39 |
| ATOM | 374 | CG  | LEU | 53 | 18.100 | 36.435 | 28.302 | 1.00 | 17.43 |
| ATOM | 375 | CD1 | LEU | 53 | 17.048 | 35.621 | 29.053 | 1.00 | 20.12 |
| ATOM | 376 | CD2 | LEU | 53 | 19.440 | 35.718 | 28.368 | 1.00 | 16.11 |
| ATOM | 377 | N   | PRO | 54 | 16.197 | 39.525 | 27.817 | 1.00 | 16.69 |
| ATOM | 378 | CA  | PRO | 54 | 16.324 | 40.962 | 28.092 | 1.00 | 18.60 |
| ATOM | 379 | C   | PRO | 54 | 17.638 | 41.414 | 28.707 | 1.00 | 25.39 |
| ATOM | 380 | O   | PRO | 54 | 17.865 | 42.609 | 28.861 | 1.00 | 18.88 |
| ATOM | 381 | CB  | PRO | 54 | 15.268 | 41.265 | 29.139 | 1.00 | 22.52 |
| ATOM | 382 | CG  | PRO | 54 | 14.832 | 39.933 | 29.720 | 1.00 | 26.02 |
| ATOM | 383 | CD  | PRO | 54 | 15.318 | 38.855 | 28.779 | 1.00 | 21.26 |
| ATOM | 384 | N   | VAL | 55 | 18.435 | 40.455 | 29.161 | 1.00 | 23.32 |
| ATOM | 385 | CA  | VAL | 55 | 19.746 | 40.716 | 29.711 | 1.00 | 15.83 |
| ATOM | 386 | C   | VAL | 55 | 20.688 | 39.868 | 28.973 | 1.00 | 19.38 |
| ATOM | 387 | O   | VAL | 55 | 20.268 | 39.035 | 28.219 | 1.00 | 20.34 |
| ATOM | 388 | CB  | VAL | 55 | 19.814 | 40.409 | 31.147 | 1.00 | 17.67 |
| ATOM | 389 | CG1 | VAL | 55 | 18.864 | 41.340 | 31.851 | 1.00 | 22.52 |
| ATOM | 390 | CG2 | VAL | 55 | 19.402 | 38.959 | 31.397 | 1.00 | 19.11 |
| ATOM | 391 | N   | PRO | 56 | 21.963 | 40.070 | 29.167 | 1.00 | 19.37 |
| ATOM | 392 | CA  | PRO | 56 | 22.911 | 39.258 | 28.447 | 1.00 | 13.09 |
| ATOM | 393 | C   | PRO | 56 | 23.059 | 37.834 | 29.038 | 1.00 | 5.83  |
| ATOM | 394 | O   | PRO | 56 | 23.067 | 37.631 | 30.254 | 1.00 | 12.35 |
| ATOM | 395 | CB  | PRO | 56 | 24.231 | 40.062 | 28.420 | 1.00 | 18.34 |
| ATOM | 396 | CG  | PRO | 56 | 23.851 | 41.478 | 28.849 | 1.00 | 20.73 |
| ATOM | 397 | CD  | PRO | 56 | 22.525 | 41.379 | 29.578 | 1.00 | 18.66 |
| ATOM | 398 | N   | TRP | 57 | 23.202 | 36.848 | 28.158 | 1.00 | 11.12 |
| ATOM | 399 | CA  | TRP | 57 | 23.354 | 35.458 | 28.595 | 1.00 | 12.55 |
| ATOM | 400 | C   | TRP | 57 | 24.411 | 35.239 | 29.700 | 1.00 | 14.13 |
| ATOM | 401 | O   | TRP | 57 | 24.178 | 34.586 | 30.709 | 1.00 | 11.49 |
| ATOM | 402 | CB  | TRP | 57 | 23.604 | 34.535 | 27.406 | 1.00 | 10.56 |
| ATOM | 403 | CG  | TRP | 57 | 22.335 | 34.237 | 26.641 | 1.00 | 12.65 |
| ATOM | 404 | CD1 | TRP | 57 | 21.999 | 34.714 | 25.426 | 1.00 | 16.24 |

**FIG. 5J**



|      |     |         |    |        |        |        |            |
|------|-----|---------|----|--------|--------|--------|------------|
| ATOM | 405 | CD2TRP  | 57 | 21.281 | 33.327 | 27.013 | 1.00 12.50 |
| ATOM | 406 | NE1 TRP | 57 | 20.784 | 34.200 | 25.018 | 1.00 14.25 |
| ATOM | 407 | CE2 TRP | 57 | 20.315 | 22.354 | 25.963 | 1.00 14.65 |
| ATOM | 408 | CE3 TRP | 57 | 21.052 | 32.521 | 28.129 | 1.00 12.01 |
| ATOM | 409 | CZ2 TRP | 57 | 19.148 | 32.583 | 26.007 | 1.00 14.36 |
| ATOM | 410 | CZ3 TRP | 57 | 19.887 | 31.767 | 28.170 | 1.00 14.23 |
| ATOM | 411 | CH2TRP  | 57 | 18.945 | 31.818 | 27.128 | 1.00 10.01 |
| ATOM | 412 | N PRO   | 58 | 25.594 | 35.800 | 29.518 | 1.00 15.78 |
| ATOM | 413 | CA PRO  | 58 | 26.629 | 35.616 | 30.503 | 1.00 9.53  |
| ATOM | 414 | C PRO   | 58 | 26.241 | 36.010 | 31.878 | 1.00 9.71  |
| ATOM | 415 | O PRO   | 58 | 26.760 | 35.467 | 32.825 | 1.00 11.70 |
| ATOM | 416 | CB PRO  | 58 | 27.833 | 36.441 | 30.040 | 1.00 10.83 |
| ATOM | 417 | CG PRO  | 58 | 27.597 | 36.748 | 28.582 | 1.00 18.50 |
| ATOM | 418 | CD PRO  | 58 | 26.137 | 36.432 | 28.278 | 1.00 15.82 |
| ATOM | 419 | N THR   | 59 | 25.336 | 36.977 | 32.021 | 1.00 7.54  |
| ATOM | 420 | CA THR  | 59 | 24.976 | 37.366 | 33.357 | 1.00 4.53  |
| ATOM | 421 | C THR   | 59 | 24.228 | 36.258 | 34.137 | 1.00 8.41  |
| ATOM | 422 | O THR   | 59 | 24.174 | 36.261 | 35.367 | 1.00 10.57 |
| ATOM | 423 | CB THR  | 59 | 24.187 | 38.691 | 33.384 | 1.00 16.64 |
| ATOM | 424 | OG1THR  | 59 | 22.895 | 38.480 | 32.844 | 1.00 15.51 |
| ATOM | 425 | CG2THR  | 59 | 24.917 | 39.731 | 32.542 | 1.00 15.76 |
| ATOM | 426 | N LEU   | 60 | 23.686 | 35.304 | 33.427 | 1.00 11.99 |
| ATOM | 427 | CA LEU  | 60 | 22.899 | 34.248 | 34.073 | 1.00 9.15  |
| ATOM | 428 | C LEU   | 60 | 23.657 | 32.944 | 34.385 | 1.00 15.62 |
| ATOM | 429 | O LEU   | 60 | 23.118 | 32.027 | 35.042 | 1.00 11.99 |
| ATOM | 430 | CB LEU  | 60 | 21.645 | 33.914 | 33.203 | 1.00 7.67  |
| ATOM | 431 | CG LEU  | 60 | 20.728 | 35.111 | 33.042 | 1.00 14.06 |
| ATOM | 432 | CD1LEU  | 60 | 19.620 | 34.775 | 32.062 | 1.00 14.54 |
| ATOM | 433 | CD2LEU  | 60 | 20.142 | 35.456 | 34.394 | 1.00 10.67 |
| ATOM | 434 | N VAL   | 61 | 24.893 | 32.837 | 33.917 | 1.00 11.27 |
| ATOM | 435 | CA VAL  | 61 | 25.656 | 31.587 | 34.094 | 1.00 4.37  |
| ATOM | 436 | C VAL   | 61 | 25.678 | 31.013 | 35.496 | 1.00 6.02  |
| ATOM | 437 | O VAL   | 61 | 25.385 | 29.805 | 35.743 | 1.00 10.75 |
| ATOM | 438 | CB VAL  | 61 | 27.050 | 31.643 | 33.406 | 1.00 7.14  |
| ATOM | 439 | CG1VAL  | 61 | 27.888 | 30.396 | 33.805 | 1.00 6.47  |
| ATOM | 440 | CG2VAL  | 61 | 26.890 | 31.745 | 31.876 | 1.00 6.63  |
| ATOM | 441 | N THR   | 62 | 26.053 | 31.843 | 36.442 | 1.00 7.02  |
| ATOM | 442 | CA THR  | 62 | 26.178 | 31.421 | 37.808 | 1.00 6.51  |
| ATOM | 443 | C THR   | 62 | 24.862 | 30.954 | 38.410 | 1.00 9.22  |
| ATOM | 444 | O THR   | 62 | 24.801 | 30.163 | 39.352 | 1.00 6.99  |
| ATOM | 445 | CB THR  | 62 | 26.816 | 32.520 | 38.660 | 1.00 16.97 |

**FIG. 5K**

|        |     |        |    |        |        |        |      |       |
|--------|-----|--------|----|--------|--------|--------|------|-------|
| ATOM   | 446 | OG1THR | 62 | 26.103 | 33.744 | 38.453 | 1.00 | 12.00 |
| ATOM   | 447 | CG2THR | 62 | 28.297 | 32.708 | 39.225 | 1.00 | 8.86  |
| ATOM   | 448 | N THR  | 63 | 23.814 | 31.547 | 37.910 | 1.00 | 9.98  |
| ATOM   | 449 | CA THR | 63 | 22.457 | 31.212 | 38.388 | 1.00 | 6.69  |
| ATOM   | 450 | C THR  | 63 | 22.033 | 29.830 | 37.865 | 1.00 | 8.14  |
| ATOM   | 451 | O THR  | 63 | 21.499 | 28.984 | 38.604 | 1.00 | 13.48 |
| ATOM   | 452 | CB THR | 63 | 21.458 | 32.312 | 37.295 | 1.00 | 11.14 |
| ATOM   | 453 | OG1THR | 63 | 21.785 | 33.498 | 38.602 | 1.00 | 11.75 |
| ATOM   | 454 | OG2THR | 63 | 20.024 | 31.897 | 38.296 | 1.00 | 9.31  |
| ATOM   | 455 | N PHE  | 64 | 22.250 | 29.620 | 36.583 | 1.00 | 10.19 |
| ATOM   | 456 | CA PHE | 64 | 21.895 | 28.371 | 35.995 | 1.00 | 8.00  |
| ATOM   | 457 | C PHE  | 64 | 22.774 | 27.253 | 36.518 | 1.00 | 25.26 |
| ATOM   | 458 | O PHE  | 64 | 23.313 | 26.147 | 36.761 | 1.00 | 9.64  |
| ATOM   | 459 | CB PHE | 64 | 22.114 | 28.438 | 34.513 | 1.00 | 6.88  |
| ATOM   | 460 | CG PHE | 64 | 21.233 | 29.357 | 33.750 | 1.00 | 10.96 |
| ATOM   | 461 | CD1PHE | 64 | 21.724 | 29.954 | 32.593 | 1.00 | 9.15  |
| ATOM   | 462 | CD2PHE | 64 | 19.899 | 29.563 | 34.106 | 1.00 | 14.43 |
| ATOM   | 463 | CE1PHE | 64 | 20.936 | 30.792 | 31.805 | 1.00 | 14.20 |
| ATOM   | 464 | CE2PHE | 64 | 19.077 | 30.375 | 33.317 | 1.00 | 13.95 |
| ATOM   | 465 | CZ PHE | 64 | 19.597 | 30.983 | 32.171 | 1.00 | 16.35 |
| HETATM | 466 | N1 CRO | 66 | 24.077 | 27.513 | 36.610 | 1.00 | 11.86 |
| HETATM | 467 | CG1CRO | 66 | 25.155 | 25.422 | 34.796 | 1.00 | 16.67 |
| HETATM | 468 | OG1CRO | 66 | 26.679 | 27.129 | 35.461 | 1.00 | 14.22 |
| HETATM | 469 | CB1CRO | 66 | 25.931 | 26.035 | 35.930 | 1.00 | 10.77 |
| HETATM | 470 | CA1CRO | 66 | 25.011 | 26.478 | 37.078 | 1.00 | 7.34  |
| HETATM | 471 | C1 CRO | 66 | 25.718 | 26.991 | 38.253 | 1.00 | 17.70 |
| HETATM | 472 | N2 CRO | 66 | 26.975 | 27.732 | 38.216 | 1.00 | 9.21  |
| HETATM | 473 | OH CRO | 66 | 32.894 | 30.804 | 36.971 | 1.00 | 13.84 |
| HETATM | 474 | CD2CRO | 66 | 30.487 | 30.110 | 39.805 | 1.00 | 10.79 |
| HETATM | 475 | CE2CRO | 66 | 31.614 | 30.563 | 39.085 | 1.00 | 10.01 |
| HETATM | 476 | CZ CRO | 66 | 31.718 | 30.300 | 37.721 | 1.00 | 9.48  |
| HETATM | 477 | CE1CRO | 66 | 30.707 | 29.546 | 37.033 | 1.00 | 17.44 |
| HETATM | 478 | CD1CRO | 66 | 29.541 | 29.103 | 37.742 | 1.00 | 11.31 |
| HETATM | 479 | CG2CRO | 66 | 29.437 | 29.370 | 39.124 | 1.00 | 7.67  |
| HETATM | 480 | CB2CRO | 66 | 28.329 | 28.822 | 39.960 | 1.00 | 10.75 |
| HETATM | 481 | CA2CRO | 66 | 27.197 | 28.245 | 39.512 | 1.00 | 16.08 |
| HETATM | 482 | C2 CRO | 66 | 26.043 | 27.875 | 40.370 | 1.00 | 5.46  |
| HETATM | 483 | O2 CRO | 66 | 26.022 | 27.962 | 41.566 | 1.00 | 13.20 |
| HETATM | 484 | N3 CRO | 66 | 25.240 | 26.978 | 39.517 | 1.00 | 18.43 |
| HETATM | 485 | CA3CRO | 66 | 23.840 | 26.511 | 39.734 | 1.00 | 10.40 |
| HETATM | 486 | C3 CRO | 66 | 23.413 | 25.550 | 40.817 | 1.00 | 11.96 |

**FIG. 5L**

|        |     |     |     |    |        |        |        |      |        |
|--------|-----|-----|-----|----|--------|--------|--------|------|--------|
| HETATM | 487 | O3  | CRO | 66 | 22.747 | 26.014 | 41.764 | 1.00 | 100.00 |
| ATOM   | 488 | N   | VAL | 68 | 23.737 | 24.208 | 41.005 | 1.00 | 29.95  |
| ATOM   | 489 | CA  | VAL | 68 | 24.209 | 22.972 | 40.304 | 1.00 | 17.16  |
| ATOM   | 490 | C   | VAL | 68 | 25.692 | 22.550 | 40.734 | 1.00 | 14.88  |
| ATOM   | 491 | O   | VAL | 68 | 26.378 | 21.821 | 40.026 | 1.00 | 9.03   |
| ATOM   | 492 | CB  | VAL | 68 | 23.870 | 22.899 | 38.831 | 1.00 | 18.94  |
| ATOM   | 493 | CG1 | VAL | 68 | 24.685 | 22.088 | 37.942 | 1.00 | 17.17  |
| ATOM   | 494 | CG2 | VAL | 68 | 22.396 | 22.538 | 38.680 | 1.00 | 18.80  |
| ATOM   | 495 | N   | GLN | 69 | 26.129 | 22.965 | 41.914 | 1.00 | 11.04  |
| ATOM   | 496 | CA  | GLN | 69 | 27.465 | 22.764 | 42.394 | 1.00 | 15.00  |
| ATOM   | 497 | C   | GLN | 69 | 27.749 | 21.366 | 42.893 | 1.00 | 22.46  |
| ATOM   | 498 | O   | GLN | 69 | 28.876 | 21.026 | 43.154 | 1.00 | 15.84  |
| ATOM   | 499 | CB  | GLN | 69 | 27.929 | 23.852 | 43.414 | 1.00 | 10.93  |
| ATOM   | 500 | CG  | GLN | 69 | 28.202 | 25.174 | 42.615 | 1.00 | 14.13  |
| ATOM   | 501 | CD  | GLN | 69 | 28.216 | 26.385 | 43.520 | 1.00 | 17.01  |
| ATOM   | 502 | OE1 | GLN | 69 | 27.433 | 26.476 | 44.448 | 1.00 | 18.94  |
| ATOM   | 503 | NE2 | GLN | 69 | 29.151 | 27.300 | 43.241 | 1.00 | 8.52   |
| ATOM   | 504 | N   | CYS | 70 | 26.703 | 20.540 | 42.906 | 1.00 | 12.10  |
| ATOM   | 505 | CA  | CYS | 70 | 26.862 | 19.171 | 43.287 | 1.00 | 11.84  |
| ATOM   | 506 | C   | CYS | 70 | 27.611 | 18.391 | 42.175 | 1.00 | 10.54  |
| ATOM   | 507 | O   | CYS | 70 | 28.036 | 17.242 | 42.367 | 1.00 | 14.70  |
| ATOM   | 508 | CB  | CYS | 70 | 25.476 | 18.584 | 43.596 | 1.00 | 14.52  |
| ATOM   | 509 | SG  | CYS | 70 | 24.325 | 19.012 | 42.251 | 1.00 | 15.61  |
| ATOM   | 510 | N   | PHE | 71 | 27.801 | 19.029 | 41.005 | 1.00 | 8.64   |
| ATOM   | 511 | CA  | PHE | 71 | 28.525 | 18.419 | 39.883 | 1.00 | 6.59   |
| ATOM   | 512 | C   | PHE | 71 | 30.041 | 18.754 | 39.876 | 1.00 | 16.43  |
| ATOM   | 513 | O   | PHE | 71 | 30.753 | 18.481 | 38.916 | 1.00 | 13.05  |
| ATOM   | 514 | CB  | PHE | 71 | 27.951 | 18.771 | 38.523 | 1.00 | 7.61   |
| ATOM   | 515 | CG  | PHE | 71 | 26.669 | 18.016 | 38.303 | 1.00 | 14.73  |
| ATOM   | 516 | CD1 | PHE | 71 | 26.693 | 16.642 | 38.050 | 1.00 | 10.34  |
| ATOM   | 517 | CD2 | PHE | 71 | 25.434 | 18.660 | 38.453 | 1.00 | 17.14  |
| ATOM   | 518 | CE1 | PHE | 71 | 25.506 | 15.931 | 37.866 | 1.00 | 15.09  |
| ATOM   | 519 | CE2 | PHE | 71 | 24.238 | 17.961 | 38.300 | 1.00 | 20.92  |
| ATOM   | 520 | CZ  | PHE | 71 | 24.282 | 16.598 | 37.990 | 1.00 | 18.49  |
| ATOM   | 521 | N   | SER | 72 | 30.500 | 19.370 | 40.938 | 1.00 | 13.13  |
| ATOM   | 522 | CA  | SER | 72 | 31.889 | 19.715 | 41.075 | 1.00 | 11.65  |
| ATOM   | 523 | C   | SER | 72 | 32.689 | 18.446 | 41.357 | 1.00 | 14.56  |
| ATOM   | 524 | O   | SER | 72 | 32.256 | 17.566 | 42.122 | 1.00 | 10.90  |
| ATOM   | 525 | CB  | SER | 72 | 32.075 | 20.672 | 42.257 | 1.00 | 8.65   |
| ATOM   | 526 | OG  | SER | 72 | 31.361 | 21.874 | 42.038 | 1.00 | 19.29  |
| ATOM   | 527 | N   | ARG | 73 | 33.905 | 18.358 | 40.794 | 1.00 | 16.27  |

**FIG. 5M**



|      |     |     |     |    |        |        |        |      |        |
|------|-----|-----|-----|----|--------|--------|--------|------|--------|
| ATOM | 569 | CB  | HIS | 77 | 42.435 | 13.806 | 50.042 | 1.00 | 19.84  |
| ATOM | 570 | CG  | HIS | 77 | 42.743 | 15.035 | 49.322 | 1.00 | 17.31  |
| ATOM | 571 | ND1 | HIS | 77 | 42.925 | 15.028 | 47.953 | 1.00 | 21.86  |
| ATOM | 572 | CD2 | HIS | 77 | 42.925 | 16.295 | 49.774 | 1.00 | 18.70  |
| ATOM | 573 | CE1 | HIS | 77 | 43.203 | 16.289 | 47.593 | 1.00 | 17.49  |
| ATOM | 574 | NE2 | HIS | 77 | 43.213 | 17.069 | 48.668 | 1.00 | 18.11  |
| ATOM | 575 | N   | MSE | 78 | 39.277 | 15.069 | 49.565 | 1.00 | 25.36  |
| ATOM | 576 | CA  | MSE | 78 | 38.412 | 16.140 | 50.026 | 1.00 | 24.65  |
| ATOM | 577 | C   | MSE | 78 | 36.920 | 15.774 | 50.066 | 1.00 | 26.47  |
| ATOM | 578 | O   | MSE | 78 | 36.070 | 16.636 | 50.260 | 1.00 | 28.16  |
| ATOM | 579 | CB  | MSE | 78 | 38.596 | 17.331 | 49.121 | 1.00 | 26.38  |
| ATOM | 580 | CG  | MSE | 78 | 39.803 | 18.177 | 49.406 | 1.00 | 27.01  |
| ATOM | 581 | SE  | MSE | 78 | 39.987 | 19.608 | 48.177 | 1.00 | 43.09  |
| ATOM | 582 | CE  | MSE | 78 | 38.874 | 20.873 | 49.044 | 1.00 | 27.11  |
| ATOM | 583 | N   | LYS | 79 | 36.606 | 14.509 | 49.856 | 1.00 | 18.68  |
| ATOM | 584 | CA  | LYS | 79 | 35.216 | 14.061 | 49.853 | 1.00 | 21.54  |
| ATOM | 585 | C   | LYS | 79 | 34.406 | 14.449 | 51.082 | 1.00 | 20.21  |
| ATOM | 586 | O   | LYS | 79 | 33.186 | 14.652 | 51.025 | 1.00 | 21.08  |
| ATOM | 587 | CB  | LYS | 79 | 35.152 | 12.581 | 49.612 | 1.00 | 23.48  |
| ATOM | 588 | CG  | LYS | 79 | 35.859 | 12.225 | 48.317 | 1.00 | 41.09  |
| ATOM | 589 | CD  | LYS | 79 | 35.159 | 11.134 | 47.535 | 1.00 | 34.66  |
| ATOM | 590 | CE  | LYS | 79 | 35.796 | 10.881 | 46.181 | 1.00 | 53.46  |
| ATOM | 591 | NZ  | LYS | 79 | 35.084 | 11.549 | 45.080 | 1.00 | 49.53  |
| ATOM | 592 | N   | ARG | 80 | 35.069 | 14.542 | 52.213 | 1.00 | 19.77  |
| ATOM | 593 | CA  | ARG | 80 | 34.365 | 14.874 | 53.434 | 1.00 | 20.13  |
| ATOM | 594 | C   | ARG | 80 | 33.898 | 16.311 | 53.481 | 1.00 | 26.42  |
| ATOM | 595 | O   | ARG | 80 | 33.251 | 16.717 | 54.467 | 1.00 | 23.51  |
| ATOM | 596 | CB  | ARG | 80 | 35.155 | 14.549 | 54.700 | 1.00 | 24.58  |
| ATOM | 597 | CG  | ARG | 80 | 36.204 | 15.620 | 55.034 | 1.00 | 29.71  |
| ATOM | 598 | CD  | ARG | 80 | 36.964 | 15.344 | 56.335 | 1.00 | 61.30  |
| ATOM | 599 | NE  | ARG | 80 | 36.551 | 16.230 | 57.415 | 1.00 | 71.14  |
| ATOM | 600 | CZ  | ARG | 80 | 37.398 | 16.882 | 58.192 | 1.00 | 100.00 |
| ATOM | 601 | NH1 | ARG | 80 | 38.714 | 16.758 | 48.040 | 1.00 | 100.00 |
| ATOM | 602 | NH2 | ARG | 80 | 36.917 | 17.679 | 59.155 | 1.00 | 99.06  |
| ATOM | 603 | N   | HIS | 81 | 34.275 | 17.121 | 52.473 | 1.00 | 18.77  |
| ATOM | 604 | CA  | HIS | 81 | 33.903 | 18.547 | 52.499 | 1.00 | 19.60  |
| ATOM | 605 | C   | HIS | 81 | 32.841 | 18.883 | 51.486 | 1.00 | 18.62  |
| ATOM | 606 | O   | HIS | 81 | 32.557 | 20.043 | 51.295 | 1.00 | 17.76  |
| ATOM | 607 | CB  | HIS | 81 | 35.129 | 19.472 | 52.283 | 1.00 | 20.39  |
| ATOM | 608 | CG  | HIS | 81 | 36.221 | 19.224 | 53.305 | 1.00 | 28.02  |
| ATOM | 609 | ND1 | HIS | 81 | 36.127 | 19.701 | 54.618 | 1.00 | 30.59  |

**FIG. 50**

|      |     |        |    |        |        |        |      |       |
|------|-----|--------|----|--------|--------|--------|------|-------|
| ATOM | 610 | CD2HIS | 81 | 37.392 | 18.535 | 53.202 | 1.00 | 29.02 |
| ATOM | 611 | CE1HIS | 81 | 37.218 | 19.308 | 55.265 | 1.00 | 26.24 |
| ATOM | 612 | NE2HIS | 81 | 37.991 | 18.603 | 54.452 | 1.00 | 28.18 |
| ATOM | 613 | N ASP  | 82 | 32.298 | 17.843 | 50.841 | 1.00 | 12.20 |
| ATOM | 614 | CA ASP | 82 | 31.358 | 18.011 | 49.769 | 1.00 | 13.24 |
| ATOM | 615 | C ASP  | 82 | 29.922 | 18.148 | 50.259 | 1.00 | 24.30 |
| ATOM | 616 | O ASP  | 82 | 29.175 | 17.195 | 50.243 | 1.00 | 16.55 |
| ATOM | 617 | CB ASP | 82 | 31.480 | 16.917 | 48.730 | 1.00 | 12.23 |
| ATOM | 618 | CG ASP | 82 | 30.642 | 17.209 | 47.518 | 1.00 | 9.92  |
| ATOM | 619 | OD1ASP | 82 | 29.870 | 18.134 | 47.459 | 1.00 | 20.31 |
| ATOM | 620 | OD2ASP | 82 | 30.938 | 16.466 | 46.507 | 1.00 | 11.12 |
| ATOM | 621 | N PHE  | 83 | 29.566 | 19.353 | 50.705 | 1.00 | 23.66 |
| ATOM | 622 | CA PHE | 83 | 28.220 | 19.634 | 51.201 | 1.00 | 20.23 |
| ATOM | 623 | C PHE  | 83 | 27.154 | 19.333 | 50.168 | 1.00 | 20.93 |
| ATOM | 624 | O PHE  | 83 | 26.116 | 18.733 | 50.503 | 1.00 | 15.97 |
| ATOM | 625 | CB PHE | 83 | 28.077 | 21.106 | 51.666 | 1.00 | 19.59 |
| ATOM | 626 | CG PHE | 83 | 26.624 | 21.613 | 51.805 | 1.00 | 16.91 |
| ATOM | 627 | CD1PHE | 83 | 25.946 | 21.498 | 53.021 | 1.00 | 17.76 |
| ATOM | 628 | CD2PHE | 83 | 25.968 | 22.236 | 50.734 | 1.00 | 18.88 |
| ATOM | 629 | CE1PHE | 83 | 24.635 | 21.960 | 53.156 | 1.00 | 24.13 |
| ATOM | 630 | CE2PHE | 83 | 24.650 | 22.690 | 50.840 | 1.00 | 19.24 |
| ATOM | 631 | CZ PHE | 83 | 24.001 | 22.575 | 52.068 | 1.00 | 20.67 |
| ATOM | 632 | N PHE  | 84 | 27.432 | 19.784 | 48.921 | 1.00 | 14.06 |
| ATOM | 633 | CA PHE | 84 | 26.515 | 19.693 | 47.809 | 1.00 | 12.96 |
| ATOM | 634 | C PHE  | 84 | 25.893 | 18.332 | 47.602 | 1.00 | 24.96 |
| ATOM | 635 | O PHE  | 84 | 24.674 | 18.200 | 47.534 | 1.00 | 21.55 |
| ATOM | 636 | CB PHE | 84 | 27.085 | 20.265 | 46.513 | 1.00 | 13.44 |
| ATOM | 637 | CG PHE | 84 | 27.630 | 21.645 | 46.721 | 1.00 | 14.27 |
| ATOM | 638 | CD1PHE | 84 | 29.001 | 21.845 | 46.890 | 1.00 | 15.17 |
| ATOM | 639 | CD2PHE | 84 | 26.781 | 22.753 | 46.752 | 1.00 | 13.48 |
| ATOM | 640 | CE1PHE | 84 | 29.520 | 23.129 | 47.073 | 1.00 | 14.63 |
| ATOM | 641 | CE2PHE | 84 | 27.276 | 24.041 | 46.969 | 1.00 | 16.34 |
| ATOM | 642 | CZ PHE | 84 | 28.650 | 24.221 | 47.137 | 1.00 | 15.77 |
| ATOM | 643 | N LYS  | 85 | 26.738 | 17.330 | 47.482 | 1.00 | 14.07 |
| ATOM | 644 | CA LYS | 85 | 26.294 | 15.985 | 47.283 | 1.00 | 13.30 |
| ATOM | 645 | C LYS  | 85 | 25.657 | 15.371 | 48.547 | 1.00 | 13.43 |
| ATOM | 646 | O LYS  | 85 | 24.773 | 14.509 | 48.429 | 1.00 | 18.46 |
| ATOM | 647 | CB LYS | 85 | 27.434 | 15.089 | 46.757 | 1.00 | 17.38 |
| ATOM | 648 | CG LYS | 85 | 27.873 | 15.372 | 45.323 | 1.00 | 13.93 |
| ATOM | 649 | CD LYS | 85 | 28.969 | 14.381 | 44.888 | 1.00 | 13.23 |
| ATOM | 650 | CE LYS | 85 | 29.766 | 14.819 | 43.662 | 1.00 | 10.36 |

**FIG. 5P**

|      |     |     |     |    |        |        |        |      |       |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|
| ATOM | 651 | NZ  | LYS | 85 | 30.319 | 16.185 | 43.773 | 1.00 | 12.92 |
| ATOM | 652 | N   | SER | 86 | 26.119 | 15.795 | 49.752 | 1.00 | 11.03 |
| ATOM | 653 | CA  | SER | 86 | 25.610 | 15.267 | 50.998 | 1.00 | 12.09 |
| ATOM | 654 | C   | SER | 86 | 24.156 | 15.639 | 51.240 | 1.00 | 21.58 |
| ATOM | 655 | O   | SER | 86 | 23.452 | 14.979 | 52.013 | 1.00 | 19.89 |
| ATOM | 656 | CB  | SER | 86 | 26.448 | 15.661 | 52.208 | 1.00 | 16.45 |
| ATOM | 657 | OG  | SER | 86 | 26.308 | 17.042 | 52.495 | 1.00 | 22.05 |
| ATOM | 658 | N   | ALA | 87 | 23.705 | 16.698 | 50.582 | 1.00 | 15.09 |
| ATOM | 659 | CA  | ALA | 87 | 22.333 | 17.138 | 50.762 | 1.00 | 19.52 |
| ATOM | 660 | C   | ALA | 87 | 21.337 | 16.399 | 49.870 | 1.00 | 18.60 |
| ATOM | 661 | O   | ALA | 87 | 20.162 | 16.557 | 50.040 | 1.00 | 19.55 |
| ATOM | 662 | CB  | ALA | 87 | 22.204 | 18.647 | 50.632 | 1.00 | 19.23 |
| ATOM | 663 | N   | MSE | 88 | 21.835 | 15.536 | 48.976 | 1.00 | 14.05 |
| ATOM | 664 | CA  | MSE | 88 | 21.007 | 14.796 | 48.035 | 1.00 | 15.32 |
| ATOM | 665 | C   | MSE | 88 | 20.496 | 13.448 | 48.579 | 1.00 | 21.48 |
| ATOM | 666 | O   | MSE | 88 | 21.109 | 12.876 | 49.457 | 1.00 | 23.03 |
| ATOM | 667 | CB  | MSE | 88 | 21.848 | 14.593 | 46.791 | 1.00 | 16.98 |
| ATOM | 668 | CG  | MSE | 88 | 22.263 | 15.891 | 46.131 | 1.00 | 10.66 |
| ATOM | 669 | SE  | MSE | 88 | 20.737 | 16.894 | 45.394 | 1.00 | 31.99 |
| ATOM | 670 | CE  | MSE | 88 | 21.318 | 18.684 | 45.748 | 1.00 | 28.86 |
| ATOM | 671 | N   | PRO | 89 | 19.363 | 12.930 | 48.084 | 1.00 | 14.78 |
| ATOM | 672 | CA  | PRO | 89 | 18.552 | 13.475 | 47.008 | 1.00 | 14.80 |
| ATOM | 673 | C   | PRO | 89 | 17.572 | 14.611 | 47.385 | 1.00 | 12.10 |
| ATOM | 674 | O   | PRO | 89 | 17.085 | 15.301 | 46.493 | 1.00 | 18.06 |
| ATOM | 675 | CB  | PRO | 89 | 17.733 | 12.294 | 46.494 | 1.00 | 17.00 |
| ATOM | 676 | CG  | PRO | 89 | 17.726 | 11.261 | 47.607 | 1.00 | 15.83 |
| ATOM | 677 | CD  | PRO | 89 | 18.844 | 11.642 | 48.560 | 1.00 | 17.16 |
| ATOM | 678 | N   | GLU | 90 | 17.278 | 14.795 | 48.695 | 1.00 | 14.63 |
| ATOM | 679 | CA  | GLU | 90 | 16.348 | 15.838 | 49.157 | 1.00 | 20.68 |
| ATOM | 680 | C   | GLU | 90 | 16.701 | 17.229 | 48.645 | 1.00 | 25.59 |
| ATOM | 681 | O   | GLU | 90 | 15.833 | 18.042 | 48.368 | 1.00 | 21.57 |
| ATOM | 682 | CB  | GLU | 90 | 16.031 | 15.816 | 50.682 | 1.00 | 22.21 |
| ATOM | 683 | CG  | GLU | 90 | 15.782 | 14.403 | 51.228 | 1.00 | 37.69 |
| ATOM | 684 | CD  | GLU | 90 | 17.071 | 13.641 | 51.447 | 1.00 | 83.49 |
| ATOM | 685 | OE1 | GLU | 90 | 18.179 | 14.151 | 51.342 | 1.00 | 54.80 |
| ATOM | 686 | OE2 | GLU | 90 | 16.875 | 12.373 | 51.749 | 1.00 | 64.65 |
| ATOM | 687 | N   | GLY | 91 | 17.977 | 17.509 | 48.510 | 1.00 | 21.39 |
| ATOM | 688 | CA  | GLY | 91 | 18.394 | 18.769 | 47.906 | 1.00 | 17.77 |
| ATOM | 689 | C   | GLY | 91 | 18.673 | 19.911 | 48.839 | 1.00 | 12.17 |
| ATOM | 690 | O   | GLY | 91 | 18.769 | 19.764 | 50.055 | 1.00 | 16.81 |
| ATOM | 691 | N   | TYR | 92 | 18.861 | 21.086 | 48.225 | 1.00 | 13.02 |

**FIG. 5Q**

|      |     |     |     |    |        |        |        |      |        |
|------|-----|-----|-----|----|--------|--------|--------|------|--------|
| ATOM | 692 | CA  | TYR | 92 | 19.143 | 22.266 | 48.994 | 1.00 | 10.33  |
| ATOM | 693 | C   | TYR | 92 | 18.575 | 23.478 | 48.347 | 1.00 | 9.87   |
| ATOM | 694 | O   | TYR | 92 | 18.270 | 23.483 | 47.144 | 1.00 | 15.89  |
| ATOM | 695 | CB  | TYR | 92 | 20.678 | 22.488 | 49.278 | 1.00 | 15.40  |
| ATOM | 696 | CG  | TYR | 92 | 21.546 | 22.468 | 48.012 | 1.00 | 15.13  |
| ATOM | 697 | CD1 | TYR | 92 | 21.620 | 23.576 | 47.166 | 1.00 | 14.75  |
| ATOM | 698 | CD2 | TYR | 92 | 22.317 | 21.350 | 47.683 | 1.00 | 16.09  |
| ATOM | 699 | CE1 | TYR | 92 | 22.404 | 23.561 | 46.006 | 1.00 | 6.50   |
| ATOM | 700 | CE2 | TYR | 92 | 23.067 | 21.300 | 46.504 | 1.00 | 15.12  |
| ATOM | 701 | CZ  | TYR | 92 | 23.156 | 22.424 | 45.683 | 1.00 | 18.13  |
| ATOM | 702 | OH  | TYR | 92 | 23.944 | 22.393 | 44.517 | 1.00 | 13.37  |
| ATOM | 703 | N   | VAL | 93 | 18.447 | 24.504 | 49.189 | 1.00 | 11.93  |
| ATOM | 704 | CA  | VAL | 93 | 18.025 | 25.822 | 48.778 | 1.00 | 14.74  |
| ATOM | 705 | C   | VAL | 93 | 19.281 | 26.666 | 48.625 | 1.00 | 16.00  |
| ATOM | 706 | O   | VAL | 93 | 20.172 | 26.625 | 49.451 | 1.00 | 16.16  |
| ATOM | 707 | CB  | VAL | 93 | 17.073 | 26.480 | 49.791 | 1.00 | 23.45  |
| ATOM | 708 | CG1 | VAL | 93 | 16.855 | 27.937 | 49.413 | 1.00 | 26.05  |
| ATOM | 709 | CG2 | VAL | 93 | 15.716 | 25.764 | 49.771 | 1.00 | 22.90  |
| ATOM | 710 | N   | GLN | 94 | 19.361 | 27.345 | 47.521 | 1.00 | 13.78  |
| ATOM | 711 | CA  | GLN | 94 | 20.480 | 28.195 | 47.227 | 1.00 | 10.53  |
| ATOM | 712 | C   | GLN | 94 | 19.948 | 29.583 | 46.998 | 1.00 | 12.23  |
| ATOM | 713 | O   | GLN | 94 | 19.153 | 29.788 | 46.061 | 1.00 | 15.52  |
| ATOM | 714 | CB  | GLN | 94 | 21.232 | 27.727 | 45.934 | 1.00 | 7.95   |
| ATOM | 715 | CG  | GLN | 94 | 22.361 | 28.708 | 45.469 | 1.00 | 11.87  |
| ATOM | 716 | CD  | GLN | 94 | 23.431 | 27.999 | 44.632 | 1.00 | 12.04  |
| ATOM | 717 | OE1 | GLN | 94 | 23.805 | 26.879 | 44.946 | 1.00 | 13.60  |
| ATOM | 718 | NE2 | GLN | 94 | 23.719 | 28.527 | 43.449 | 1.00 | 7.98   |
| ATOM | 719 | N   | GLU | 95 | 20.396 | 30.531 | 47.820 | 1.00 | 11.78  |
| ATOM | 720 | CA  | GLU | 95 | 19.974 | 31.899 | 47.643 | 1.00 | 13.47  |
| ATOM | 721 | C   | GLU | 95 | 21.149 | 32.804 | 47.398 | 1.00 | 18.42  |
| ATOM | 722 | O   | GLU | 95 | 22.206 | 32.623 | 47.985 | 1.00 | 19.23  |
| ATOM | 723 | CB  | GLU | 95 | 19.277 | 32.427 | 48.878 | 1.00 | 13.52  |
| ATOM | 724 | CG  | GLU | 95 | 18.009 | 31.684 | 49.215 | 1.00 | 28.46  |
| ATOM | 725 | CD  | GLU | 95 | 17.657 | 32.016 | 50.622 | 1.00 | 45.93  |
| ATOM | 726 | OE1 | GLU | 95 | 17.574 | 33.166 | 51.011 | 1.00 | 100.00 |
| ATOM | 727 | OE2 | GLU | 95 | 17.764 | 30.987 | 51.423 | 1.00 | 61.33  |
| ATOM | 728 | N   | ARG | 96 | 20.929 | 33.838 | 46.601 | 1.00 | 16.51  |
| ATOM | 729 | CA  | ARG | 96 | 21.978 | 34.783 | 46.342 | 1.00 | 16.87  |
| ATOM | 730 | C   | ARG | 96 | 21.510 | 36.195 | 46.206 | 1.00 | 15.84  |
| ATOM | 731 | O   | ARG | 96 | 20.389 | 36.488 | 45.806 | 1.00 | 15.01  |
| ATOM | 732 | CB  | ARG | 96 | 22.582 | 34.463 | 44.967 | 1.00 | 16.19  |

**FIG. 5R**



|      |     |     |     |     |        |        |        |      |       |
|------|-----|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 733 | CG  | ARG | 96  | 23.495 | 33.247 | 44.929 | 1.00 | 17.61 |
| ATOM | 734 | CD  | ARG | 96  | 24.615 | 33.453 | 43.908 | 1.00 | 9.06  |
| ATOM | 735 | NE  | ARG | 96  | 25.411 | 32.277 | 43.766 | 1.00 | 9.88  |
| ATOM | 736 | CZ  | ARG | 96  | 25.434 | 31.493 | 42.693 | 1.00 | 20.03 |
| ATOM | 737 | NH1 | ARG | 96  | 24.684 | 31.709 | 41.615 | 1.00 | 15.29 |
| ATOM | 738 | NH2 | ARG | 96  | 26.236 | 30.430 | 42.714 | 1.00 | 11.03 |
| ATOM | 739 | N   | THR | 97  | 22.470 | 37.068 | 46.344 | 1.00 | 13.39 |
| ATOM | 740 | CA  | THR | 97  | 22.368 | 38.424 | 45.935 | 1.00 | 13.12 |
| ATOM | 741 | C   | THR | 97  | 23.593 | 38.688 | 45.084 | 1.00 | 16.81 |
| ATOM | 742 | O   | THR | 97  | 24.686 | 38.347 | 45.485 | 1.00 | 19.25 |
| ATOM | 743 | CB  | THR | 97  | 22.282 | 39.442 | 47.066 | 1.00 | 26.27 |
| ATOM | 744 | OG1 | THR | 97  | 21.225 | 39.101 | 47.945 | 1.00 | 31.43 |
| ATOM | 745 | CG2 | THR | 97  | 22.038 | 40.804 | 46.445 | 1.00 | 15.90 |
| ATOM | 746 | N   | ILE | 98  | 23.396 | 39.219 | 43.899 | 1.00 | 16.23 |
| ATOM | 747 | CA  | ILE | 98  | 24.486 | 39.526 | 42.977 | 1.00 | 16.70 |
| ATOM | 748 | C   | ILE | 98  | 24.533 | 41.017 | 42.686 | 1.00 | 21.10 |
| ATOM | 749 | O   | ILE | 98  | 23.628 | 41.566 | 42.075 | 1.00 | 14.58 |
| ATOM | 750 | CB  | ILE | 98  | 24.385 | 38.752 | 41.660 | 1.00 | 13.47 |
| ATOM | 751 | CG1 | ILE | 98  | 24.480 | 37.236 | 41.890 | 1.00 | 16.09 |
| ATOM | 752 | CG2 | ILE | 98  | 25.457 | 39.231 | 40.679 | 1.00 | 13.30 |
| ATOM | 753 | CD1 | ILE | 98  | 23.875 | 36.431 | 40.738 | 1.00 | 13.93 |
| ATOM | 754 | N   | PHE | 99  | 25.613 | 41.678 | 43.110 | 1.00 | 14.86 |
| ATOM | 755 | CA  | PHE | 99  | 25.719 | 43.098 | 42.896 | 1.00 | 12.44 |
| ATOM | 756 | C   | PHE | 99  | 26.514 | 43.441 | 41.699 | 1.00 | 20.37 |
| ATOM | 757 | O   | PHE | 99  | 27.696 | 43.164 | 41.700 | 1.00 | 20.07 |
| ATOM | 758 | CB  | PHE | 99  | 26.401 | 43.770 | 44.084 | 1.00 | 15.96 |
| ATOM | 759 | CG  | PHE | 99  | 25.638 | 43.624 | 45.356 | 1.00 | 21.41 |
| ATOM | 760 | CD1 | PHE | 99  | 25.863 | 42.524 | 46.189 | 1.00 | 24.98 |
| ATOM | 761 | CD2 | PHE | 99  | 24.698 | 44.585 | 45.743 | 1.00 | 22.94 |
| ATOM | 762 | CE1 | PHE | 99  | 25.176 | 42.400 | 47.400 | 1.00 | 32.06 |
| ATOM | 763 | CE2 | PHE | 99  | 23.992 | 44.469 | 46.946 | 1.00 | 24.26 |
| ATOM | 764 | CZ  | PHE | 99  | 24.235 | 43.369 | 47.771 | 1.00 | 28.19 |
| ATOM | 765 | N   | PHE | 100 | 25.906 | 44.085 | 40.704 | 1.00 | 12.53 |
| ATOM | 766 | CA  | PHE | 100 | 26.679 | 44.522 | 39.554 | 1.00 | 8.75  |
| ATOM | 767 | C   | PHE | 100 | 27.294 | 45.855 | 39.872 | 1.00 | 21.81 |
| ATOM | 768 | O   | PHE | 100 | 26.599 | 46.775 | 40.308 | 1.00 | 20.31 |
| ATOM | 769 | CB  | PHE | 100 | 25.927 | 44.572 | 38.226 | 1.00 | 5.94  |
| ATOM | 770 | CG  | PHE | 100 | 25.537 | 43.183 | 37.764 | 1.00 | 12.75 |
| ATOM | 771 | CD1 | PHE | 100 | 24.426 | 42.538 | 38.325 | 1.00 | 16.31 |
| ATOM | 772 | CD2 | PHE | 100 | 26.317 | 42.484 | 36.843 | 1.00 | 15.27 |
| ATOM | 773 | CE1 | PHE | 100 | 24.087 | 41.230 | 37.975 | 1.00 | 13.50 |

**FIG. 5S**

|      |     |         |     |        |        |        |      |       |
|------|-----|---------|-----|--------|--------|--------|------|-------|
| ATOM | 774 | CE2 PHE | 100 | 25.965 | 41.192 | 36.435 | 1.00 | 21.25 |
| ATOM | 775 | CZ PHE  | 100 | 24.852 | 40.567 | 37.014 | 1.00 | 21.06 |
| ATOM | 776 | N LYS   | 101 | 28.603 | 45.946 | 39.737 | 1.00 | 15.49 |
| ATOM | 777 | CA LYS  | 101 | 29.270 | 47.179 | 40.085 | 1.00 | 17.93 |
| ATOM | 778 | C LYS   | 101 | 28.732 | 48.349 | 39.287 | 1.00 | 13.71 |
| ATOM | 779 | O LYS   | 101 | 28.658 | 48.304 | 38.072 | 1.00 | 17.18 |
| ATOM | 780 | CB LYS  | 101 | 30.784 | 47.069 | 39.950 | 1.00 | 17.13 |
| ATOM | 781 | CG LYS  | 101 | 31.518 | 48.252 | 40.551 | 1.00 | 18.01 |
| ATOM | 782 | CD LYS  | 101 | 33.036 | 48.060 | 40.534 | 1.00 | 26.70 |
| ATOM | 783 | CE LYS  | 101 | 33.797 | 49.116 | 41.332 | 1.00 | 41.58 |
| ATOM | 784 | N ASP   | 102 | 28.353 | 49.403 | 39.997 | 1.00 | 18.09 |
| ATOM | 785 | CA ASP  | 102 | 27.805 | 50.618 | 39.368 | 1.00 | 23.08 |
| ATOM | 786 | C ASP   | 102 | 26.559 | 50.356 | 38.549 | 1.00 | 25.42 |
| ATOM | 787 | O ASP   | 102 | 26.292 | 51.061 | 37.586 | 1.00 | 23.34 |
| ATOM | 788 | CB ASP  | 102 | 28.840 | 51.369 | 38.516 | 1.00 | 26.27 |
| ATOM | 789 | CG ASP  | 102 | 30.109 | 51.629 | 39.296 | 1.00 | 57.01 |
| ATOM | 790 | OD1ASP  | 102 | 31.206 | 51.233 | 38.931 | 1.00 | 63.33 |
| ATOM | 791 | OD2ASP  | 102 | 29.886 | 52.200 | 40.464 | 1.00 | 47.66 |
| ATOM | 792 | N ASP   | 103 | 25.813 | 49.328 | 38.933 | 1.00 | 20.17 |
| ATOM | 793 | CA ASP  | 103 | 24.602 | 48.949 | 38.233 | 1.00 | 15.70 |
| ATOM | 794 | C ASP   | 103 | 23.608 | 48.284 | 39.189 | 1.00 | 18.47 |
| ATOM | 795 | O ASP   | 103 | 23.749 | 48.431 | 40.409 | 1.00 | 17.72 |
| ATOM | 796 | CB ASP  | 103 | 24.899 | 48.085 | 36.995 | 1.00 | 19.89 |
| ATOM | 797 | CG ASP  | 103 | 23.946 | 48.387 | 35.860 | 1.00 | 23.93 |
| ATOM | 798 | OD1ASP  | 103 | 24.238 | 48.274 | 34.688 | 1.00 | 19.05 |
| ATOM | 799 | OD2ASP  | 103 | 22.774 | 48.809 | 36.283 | 1.00 | 23.89 |
| ATOM | 800 | N GLY   | 104 | 22.612 | 47.542 | 38.646 | 1.00 | 20.17 |
| ATOM | 801 | CA GLY  | 104 | 21.598 | 46.900 | 39.498 | 1.00 | 20.22 |
| ATOM | 802 | C GLY   | 104 | 22.055 | 45.619 | 40.180 | 1.00 | 24.68 |
| ATOM | 803 | O GLY   | 104 | 23.202 | 45.211 | 40.085 | 1.00 | 18.06 |
| ATOM | 804 | N ASN   | 105 | 21.125 | 44.967 | 40.872 | 1.00 | 15.71 |
| ATOM | 805 | CA ASN  | 105 | 21.425 | 43.703 | 41.510 | 1.00 | 8.89  |
| ATOM | 806 | C ASN   | 105 | 20.399 | 42.620 | 41.181 | 1.00 | 21.85 |
| ATOM | 807 | O ASN   | 105 | 19.255 | 42.911 | 40.824 | 1.00 | 15.17 |
| ATOM | 808 | CB ASN  | 105 | 21.605 | 43.840 | 43.001 | 1.00 | 8.58  |
| ATOM | 809 | CG ASN  | 105 | 20.359 | 44.366 | 43.697 | 1.00 | 43.57 |
| ATOM | 810 | OD1ASN  | 105 | 19.565 | 43.601 | 44.259 | 1.00 | 36.67 |
| ATOM | 811 | ND2ASN  | 105 | 20.178 | 45.674 | 43.659 | 1.00 | 36.47 |
| ATOM | 812 | N TYR   | 106 | 20.826 | 41.365 | 41.328 | 1.00 | 16.80 |
| ATOM | 813 | CA TYR  | 106 | 19.966 | 40.219 | 41.156 | 1.00 | 13.90 |
| ATOM | 814 | C TYR   | 106 | 19.763 | 39.543 | 42.475 | 1.00 | 11.05 |

**FIG. 5T**

|      |     |     |     |     |        |        |        |      |       |
|------|-----|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 815 | O   | TYR | 106 | 20.678 | 39.404 | 43.281 | 1.00 | 13.86 |
| ATOM | 816 | CB  | TYR | 106 | 20.547 | 39.128 | 40.246 | 1.00 | 15.88 |
| ATOM | 817 | CG  | TYR | 106 | 20.619 | 39.398 | 38.793 | 1.00 | 15.57 |
| ATOM | 818 | CD1 | TYR | 106 | 19.952 | 40.458 | 38.178 | 1.00 | 13.14 |
| ATOM | 819 | CD2 | TYR | 106 | 21.373 | 38.524 | 38.006 | 1.00 | 13.35 |
| ATOM | 820 | CE1 | TYR | 106 | 20.038 | 40.632 | 36.793 | 1.00 | 13.44 |
| ATOM | 821 | CE2 | TYR | 106 | 21.481 | 38.692 | 36.628 | 1.00 | 10.87 |
| ATOM | 822 | CZ  | TYR | 106 | 20.814 | 39.751 | 36.025 | 1.00 | 15.93 |
| ATOM | 823 | OH  | TYR | 106 | 20.970 | 39.931 | 34.670 | 1.00 | 17.32 |
| ATOM | 824 | N   | LYS | 107 | 18.538 | 39.115 | 42.709 | 1.00 | 12.39 |
| ATOM | 825 | CA  | LYS | 107 | 18.194 | 38.349 | 43.897 | 1.00 | 11.51 |
| ATOM | 826 | C   | LYS | 107 | 17.619 | 37.037 | 43.397 | 1.00 | 17.25 |
| ATOM | 827 | O   | LYS | 107 | 16.704 | 37.010 | 42.562 | 1.00 | 13.14 |
| ATOM | 828 | CB  | LYS | 107 | 17.217 | 39.063 | 44.823 | 1.00 | 14.82 |
| ATOM | 829 | CG  | LYS | 107 | 17.860 | 39.631 | 46.060 | 1.00 | 40.71 |
| ATOM | 830 | CD  | LYS | 107 | 18.528 | 40.974 | 45.793 | 1.00 | 43.48 |
| ATOM | 831 | N   | THR | 108 | 18.205 | 35.951 | 43.835 | 1.00 | 14.95 |
| ATOM | 832 | CA  | THR | 108 | 17.774 | 34.658 | 43.352 | 1.00 | 11.97 |
| ATOM | 833 | C   | THR | 108 | 17.463 | 33.696 | 44.468 | 1.00 | 15.81 |
| ATOM | 834 | O   | THR | 108 | 18.043 | 33.734 | 45.582 | 1.00 | 18.68 |
| ATOM | 835 | CB  | THR | 108 | 18.847 | 34.034 | 42.410 | 1.00 | 23.81 |
| ATOM | 836 | OG1 | THR | 108 | 20.064 | 33.791 | 43.137 | 1.00 | 13.88 |
| ATOM | 837 | CG2 | THR | 108 | 19.123 | 34.968 | 41.264 | 1.00 | 13.04 |
| ATOM | 838 | N   | ARG | 109 | 16.560 | 32.804 | 44.154 | 1.00 | 13.57 |
| ATOM | 839 | CA  | ARG | 109 | 16.212 | 31.751 | 45.048 | 1.00 | 12.56 |
| ATOM | 840 | C   | ARG | 109 | 15.939 | 30.498 | 44.254 | 1.00 | 13.07 |
| ATOM | 841 | O   | ARG | 109 | 15.239 | 30.509 | 43.249 | 1.00 | 12.52 |
| ATOM | 842 | CB  | ARG | 109 | 15.069 | 32.100 | 45.959 | 1.00 | 17.32 |
| ATOM | 843 | CG  | ARG | 109 | 14.767 | 30.995 | 46.932 | 1.00 | 17.92 |
| ATOM | 844 | CD  | ARG | 109 | 13.400 | 31.160 | 47.610 | 1.00 | 19.99 |
| ATOM | 845 | NE  | ARG | 109 | 12.821 | 29.854 | 47.883 | 1.00 | 36.05 |
| ATOM | 846 | CZ  | ARG | 109 | 12.968 | 29.244 | 49.035 | 1.00 | 55.71 |
| ATOM | 847 | NH1 | ARG | 109 | 13.630 | 29.815 | 50.046 | 1.00 | 44.11 |
| ATOM | 848 | NH2 | ARG | 109 | 12.432 | 28.041 | 49.195 | 1.00 | 94.34 |
| ATOM | 849 | N   | ALA | 110 | 16.577 | 29.414 | 44.635 | 1.00 | 13.26 |
| ATOM | 850 | CA  | ALA | 110 | 16.377 | 28.207 | 43.870 | 1.00 | 12.68 |
| ATOM | 851 | C   | ALA | 110 | 16.346 | 26.979 | 44.734 | 1.00 | 13.15 |
| ATOM | 852 | O   | ALA | 110 | 16.829 | 26.965 | 45.869 | 1.00 | 16.75 |
| ATOM | 853 | CB  | ALA | 110 | 17.465 | 28.059 | 42.822 | 1.00 | 17.31 |
| ATOM | 854 | N   | GLU | 111 | 15.770 | 25.939 | 44.176 | 1.00 | 15.39 |
| ATOM | 855 | CA  | GLU | 111 | 15.741 | 24.655 | 44.823 | 1.00 | 15.24 |

**FIG. 5U**

|      |     |     |     |     |        |        |        |      |        |
|------|-----|-----|-----|-----|--------|--------|--------|------|--------|
| ATOM | 856 | C   | GLU | 111 | 16.438 | 23.678 | 43.926 | 1.00 | 12.08  |
| ATOM | 857 | O   | GLU | 111 | 16.086 | 23.545 | 42.771 | 1.00 | 15.70  |
| ATOM | 858 | CB  | GLU | 111 | 14.303 | 24.123 | 44.993 | 1.00 | 19.20  |
| ATOM | 859 | CG  | GLU | 111 | 13.744 | 24.242 | 46.399 | 1.00 | 38.62  |
| ATOM | 860 | CD  | GLU | 111 | 12.247 | 24.280 | 46.372 | 1.00 | 60.99  |
| ATOM | 861 | OE1 | GLU | 111 | 11.589 | 23.843 | 45.432 | 1.00 | 76.05  |
| ATOM | 862 | OE2 | GLU | 111 | 11.742 | 24.956 | 47.380 | 1.00 | 54.87  |
| ATOM | 863 | N   | VAL | 112 | 17.438 | 22.965 | 44.457 | 1.00 | 10.78  |
| ATOM | 864 | CA  | VAL | 112 | 18.063 | 21.978 | 43.631 | 1.00 | 10.98  |
| ATOM | 865 | C   | VAL | 112 | 17.968 | 20.630 | 44.261 | 1.00 | 8.62   |
| ATOM | 866 | O   | VAL | 112 | 18.271 | 20.438 | 45.432 | 1.00 | 15.63  |
| ATOM | 867 | CB  | VAL | 112 | 19.428 | 22.358 | 43.012 | 1.00 | 22.75  |
| ATOM | 868 | CG1 | VAL | 112 | 19.966 | 23.704 | 43.487 | 1.00 | 16.69  |
| ATOM | 869 | CG2 | VAL | 112 | 20.452 | 21.232 | 43.078 | 1.00 | 18.47  |
| ATOM | 870 | N   | LYS | 113 | 17.415 | 19.732 | 43.516 | 1.00 | 14.67  |
| ATOM | 871 | CA  | LYS | 113 | 17.175 | 18.421 | 44.045 | 1.00 | 16.41  |
| ATOM | 872 | C   | LYS | 113 | 16.822 | 17.485 | 42.931 | 1.00 | 7.11   |
| ATOM | 873 | O   | LYS | 113 | 16.695 | 17.893 | 41.808 | 1.00 | 16.27  |
| ATOM | 874 | CB  | LYS | 113 | 16.032 | 18.497 | 45.036 | 1.00 | 22.50  |
| ATOM | 875 | CG  | LYS | 113 | 14.792 | 19.084 | 44.376 | 1.00 | 20.40  |
| ATOM | 876 | CD  | LYS | 113 | 13.509 | 18.321 | 44.703 | 1.00 | 44.65  |
| ATOM | 877 | CE  | LYS | 113 | 12.526 | 19.134 | 45.528 | 1.00 | 54.02  |
| ATOM | 878 | NZ  | LYS | 113 | 12.379 | 20.518 | 45.036 | 1.00 | 100.00 |
| ATOM | 879 | N   | PHE | 114 | 16.683 | 16.208 | 43.267 | 1.00 | 10.09  |
| ATOM | 880 | CA  | PHE | 114 | 16.325 | 15.175 | 42.317 | 1.00 | 11.41  |
| ATOM | 881 | C   | PHE | 114 | 14.806 | 14.975 | 42.181 | 1.00 | 14.18  |
| ATOM | 882 | O   | PHE | 114 | 14.110 | 14.878 | 43.160 | 1.00 | 15.03  |
| ATOM | 883 | CB  | PHE | 114 | 16.866 | 13.838 | 42.838 | 1.00 | 12.89  |
| ATOM | 884 | CG  | PHE | 114 | 18.231 | 13.536 | 42.338 | 1.00 | 16.80  |
| ATOM | 885 | CD1 | PHE | 114 | 19.344 | 13.795 | 43.139 | 1.00 | 18.61  |
| ATOM | 886 | CD2 | PHE | 114 | 18.403 | 13.009 | 41.056 | 1.00 | 19.50  |
| ATOM | 887 | CE1 | PHE | 114 | 20.627 | 13.500 | 42.665 | 1.00 | 22.78  |
| ATOM | 888 | CE2 | PHE | 114 | 19.673 | 12.708 | 40.572 | 1.00 | 25.36  |
| ATOM | 889 | CZ  | PHE | 114 | 20.780 | 12.953 | 41.387 | 1.00 | 23.99  |
| ATOM | 890 | N   | GLU | 115 | 14.354 | 14.819 | 40.966 | 1.00 | 15.29  |
| ATOM | 891 | CA  | GLU | 115 | 12.978 | 14.473 | 40.642 | 1.00 | 11.40  |
| ATOM | 892 | C   | GLU | 115 | 13.121 | 13.193 | 39.906 | 1.00 | 13.30  |
| ATOM | 893 | O   | GLU | 115 | 13.434 | 13.207 | 38.730 | 1.00 | 18.72  |
| ATOM | 894 | CB  | GLU | 115 | 12.348 | 15.481 | 39.667 | 1.00 | 9.68   |
| ATOM | 895 | CG  | GLU | 115 | 11.856 | 16.747 | 40.376 | 1.00 | 19.54  |
| ATOM | 896 | CD  | GLU | 115 | 10.742 | 16.460 | 41.342 | 1.00 | 38.12  |

**FIG. 5V**

|      |     |         |     |        |        |        |            |
|------|-----|---------|-----|--------|--------|--------|------------|
| ATOM | 897 | OE1 GLU | 115 | 10.181 | 15.395 | 41.431 | 1.00 34.84 |
| ATOM | 898 | OE2 GLU | 115 | 10.460 | 17.461 | 42.079 | 1.00 27.88 |
| ATOM | 899 | N GLY   | 116 | 13.005 | 12.087 | 40.585 | 1.00 14.51 |
| ATOM | 900 | CA GLY  | 116 | 13.225 | 10.861 | 39.869 | 1.00 15.91 |
| ATOM | 901 | C GLY   | 116 | 14.727 | 10.767 | 39.641 | 1.00 23.59 |
| ATOM | 902 | O GLY   | 116 | 15.516 | 10.922 | 40.570 | 1.00 19.35 |
| ATOM | 903 | N ASP   | 117 | 15.137 | 10.564 | 38.439 | 1.00 20.26 |
| ATOM | 904 | CA ASP  | 117 | 16.572 | 10.462 | 38.233 | 1.00 28.00 |
| ATOM | 905 | C ASP   | 117 | 17.237 | 11.677 | 37.598 | 1.00 22.39 |
| ATOM | 906 | O ASP   | 117 | 18.423 | 11.672 | 37.265 | 1.00 21.38 |
| ATOM | 907 | CB ASP  | 117 | 17.055 | 9.074  | 37.733 | 1.00 33.06 |
| ATOM | 908 | CG ASP  | 117 | 16.624 | 8.677  | 36.348 | 1.00 55.04 |
| ATOM | 909 | OD1ASP  | 117 | 16.230 | 9.468  | 35.495 | 1.00 59.57 |
| ATOM | 910 | OD2ASP  | 117 | 16.805 | 7.391  | 36.130 | 1.00 82.48 |
| ATOM | 911 | N THR   | 118 | 16.463 | 12.729 | 37.493 | 1.00 19.62 |
| ATOM | 912 | CA THR  | 118 | 16.889 | 13.981 | 36.910 | 1.00 18.21 |
| ATOM | 913 | C THR   | 118 | 17.186 | 14.988 | 37.976 | 1.00 18.92 |
| ATOM | 914 | O THR   | 118 | 16.498 | 15.064 | 38.996 | 1.00 15.94 |
| ATOM | 915 | CB THR  | 118 | 15.806 | 14.497 | 35.952 | 1.00 19.03 |
| ATOM | 916 | OG1THR  | 118 | 15.552 | 13.508 | 34.990 | 1.00 21.42 |
| ATOM | 917 | CG2THR  | 118 | 16.217 | 15.793 | 35.275 | 1.00 15.49 |
| ATOM | 918 | N LEU   | 119 | 18.284 | 15.681 | 37.805 | 1.00 13.66 |
| ATOM | 919 | CA LEU  | 119 | 18.679 | 16.706 | 38.759 | 1.00 13.50 |
| ATOM | 920 | C LEU   | 119 | 18.036 | 17.992 | 38.269 | 1.00 8.81  |
| ATOM | 921 | O LEU   | 119 | 18.194 | 18.368 | 37.091 | 1.00 12.49 |
| ATOM | 922 | CB LEU  | 119 | 20.243 | 16.815 | 38.839 | 1.00 12.25 |
| ATOM | 923 | CG LEU  | 119 | 20.845 | 17.678 | 39.951 | 1.00 3.90  |
| ATOM | 924 | CD1LEU  | 119 | 20.701 | 19.167 | 39.669 | 1.00 10.11 |
| ATOM | 925 | CD2LEU  | 119 | 20.366 | 17.311 | 41.333 | 1.00 7.86  |
| ATOM | 926 | N VAL   | 120 | 17.230 | 18.595 | 39.170 | 1.00 13.34 |
| ATOM | 927 | CA VAL  | 120 | 16.466 | 19.797 | 38.859 | 1.00 13.77 |
| ATOM | 928 | C VAL   | 120 | 16.929 | 21.039 | 39.587 | 1.00 8.56  |
| ATOM | 929 | O VAL   | 120 | 17.135 | 21.039 | 40.762 | 1.00 13.32 |
| ATOM | 930 | CB VAL  | 120 | 14.939 | 19.566 | 39.082 | 1.00 17.60 |
| ATOM | 931 | CG1VAL  | 120 | 14.133 | 20.790 | 38.642 | 1.00 17.58 |
| ATOM | 932 | CG2VAL  | 120 | 14.501 | 18.351 | 38.246 | 1.00 15.35 |
| ATOM | 933 | N ASN   | 121 | 17.067 | 22.111 | 38.839 | 1.00 12.24 |
| ATOM | 934 | CA ASN  | 121 | 17.424 | 23.405 | 39.400 | 1.00 11.78 |
| ATOM | 935 | C ASN   | 121 | 16.301 | 24.382 | 39.060 | 1.00 11.18 |
| ATOM | 936 | O ASN   | 121 | 16.195 | 24.802 | 37.934 | 1.00 11.09 |
| ATOM | 937 | CB ASN  | 121 | 18.753 | 23.928 | 38.791 | 1.00 11.41 |

**FIG. 5W**

|      |     |     |     |     |        |        |        |      |       |
|------|-----|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 938 | CG  | ASN | 121 | 19.201 | 25.261 | 39.367 | 1.00 | 11.07 |
| ATOM | 939 | OD  | ASN | 121 | 18.773 | 25.654 | 40.461 | 1.00 | 12.06 |
| ATOM | 940 | ND2 | ASN | 121 | 20.124 | 25.938 | 38.670 | 1.00 | 11.90 |
| ATOM | 941 | N   | ARG | 122 | 15.470 | 24.706 | 40.029 | 1.00 | 13.69 |
| ATOM | 942 | CA  | ARG | 122 | 14.348 | 25.610 | 39.825 | 1.00 | 12.99 |
| ATOM | 943 | C   | ARG | 122 | 14.622 | 26.946 | 40.498 | 1.00 | 5.89  |
| ATOM | 944 | O   | ARG | 122 | 14.749 | 27.011 | 41.723 | 1.00 | 14.47 |
| ATOM | 945 | CB  | ARG | 122 | 13.068 | 25.025 | 40.417 | 1.00 | 15.99 |
| ATOM | 946 | CG  | ARG | 122 | 12.478 | 23.921 | 39.589 | 1.00 | 30.23 |
| ATOM | 947 | CD  | ARG | 122 | 11.282 | 23.244 | 40.281 | 1.00 | 60.61 |
| ATOM | 948 | N   | ILE | 123 | 14.663 | 27.992 | 39.680 | 1.00 | 11.46 |
| ATOM | 949 | CA  | ILE | 123 | 15.030 | 29.340 | 40.095 | 1.00 | 11.86 |
| ATOM | 950 | C   | ILE | 123 | 13.991 | 30.450 | 39.835 | 1.00 | 10.54 |
| ATOM | 951 | O   | ILE | 123 | 13.370 | 30.535 | 38.765 | 1.00 | 12.83 |
| ATOM | 952 | CB  | ILE | 123 | 16.296 | 29.757 | 39.292 | 1.00 | 15.41 |
| ATOM | 953 | CG1 | ILE | 123 | 17.316 | 28.585 | 39.180 | 1.00 | 12.27 |
| ATOM | 954 | CG2 | ILE | 123 | 16.944 | 30.993 | 39.918 | 1.00 | 14.01 |
| ATOM | 955 | CD1 | ILE | 123 | 17.652 | 28.242 | 37.743 | 1.00 | 7.74  |
| ATOM | 956 | N   | GLU | 124 | 13.953 | 31.358 | 40.793 | 1.00 | 11.36 |
| ATOM | 957 | CA  | GLU | 124 | 13.189 | 32.752 | 40.700 | 1.00 | 15.20 |
| ATOM | 958 | C   | GLU | 124 | 14.168 | 33.713 | 40.811 | 1.00 | 11.93 |
| ATOM | 959 | O   | GLU | 124 | 14.919 | 33.797 | 41.780 | 1.00 | 15.61 |
| ATOM | 960 | CB  | GLU | 124 | 12.028 | 32.677 | 41.751 | 1.00 | 19.74 |
| ATOM | 961 | CG  | GLU | 124 | 12.387 | 33.337 | 43.089 | 1.00 | 72.94 |
| ATOM | 962 | N   | LEU | 125 | 14.183 | 34.550 | 39.808 | 1.00 | 12.19 |
| ATOM | 963 | CA  | LEU | 125 | 15.092 | 35.654 | 39.767 | 1.00 | 15.00 |
| ATOM | 964 | C   | LEU | 125 | 14.420 | 37.011 | 39.722 | 1.00 | 19.35 |
| ATOM | 965 | O   | LEU | 125 | 13.563 | 37.267 | 38.893 | 1.00 | 18.41 |
| ATOM | 966 | CB  | LEU | 125 | 15.976 | 35.533 | 38.510 | 1.00 | 14.29 |
| ATOM | 967 | CG  | LEU | 125 | 17.003 | 36.683 | 38.375 | 1.00 | 17.65 |
| ATOM | 968 | CD1 | LEU | 125 | 18.302 | 36.083 | 37.849 | 1.00 | 13.46 |
| ATOM | 969 | CD2 | LEU | 125 | 16.511 | 37.732 | 37.367 | 1.00 | 12.09 |
| ATOM | 970 | N   | LYS | 126 | 14.890 | 37.897 | 40.554 | 1.00 | 12.73 |
| ATOM | 971 | CA  | LYS | 126 | 14.391 | 39.260 | 40.579 | 1.00 | 15.92 |
| ATOM | 972 | C   | LYS | 126 | 15.563 | 40.276 | 40.445 | 1.00 | 18.53 |
| ATOM | 973 | O   | LYS | 126 | 16.489 | 40.246 | 41.246 | 1.00 | 19.86 |
| ATOM | 974 | CB  | LYS | 126 | 13.611 | 39.487 | 41.877 | 1.00 | 17.31 |
| ATOM | 975 | CG  | LYS | 126 | 12.853 | 40.786 | 41.923 | 1.00 | 33.94 |
| ATOM | 976 | CD  | LYS | 126 | 11.366 | 40.601 | 41.675 | 1.00 | 60.87 |
| ATOM | 977 | CE  | LYS | 126 | 10.652 | 41.929 | 41.521 | 1.00 | 52.70 |
| ATOM | 978 | NZ  | LYS | 126 | 11.229 | 42.988 | 42.367 | 1.00 | 47.22 |

**FIG. 5X**

|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 979  | N   | GLY | 127 | 15.514 | 41.127 | 39.411 | 1.00 | 18.71 |
| ATOM | 980  | CA  | GLY | 127 | 16.551 | 42.151 | 39.121 | 1.00 | 17.32 |
| ATOM | 981  | C   | GLY | 127 | 16.012 | 43.572 | 39.272 | 1.00 | 25.32 |
| ATOM | 982  | O   | GLY | 127 | 14.981 | 43.908 | 38.693 | 1.00 | 20.14 |
| ATOM | 983  | N   | ILE | 128 | 16.706 | 44.404 | 40.070 | 1.00 | 18.42 |
| ATOM | 984  | CA  | ILE | 128 | 16.282 | 45.787 | 40.243 | 1.00 | 21.04 |
| ATOM | 985  | C   | ILE | 128 | 17.405 | 46.789 | 40.196 | 1.00 | 25.93 |
| ATOM | 986  | O   | ILE | 128 | 18.562 | 46.496 | 40.429 | 1.00 | 19.37 |
| ATOM | 987  | CB  | ILE | 128 | 15.482 | 46.052 | 41.504 | 1.00 | 23.82 |
| ATOM | 988  | CG1 | ILE | 128 | 16.408 | 45.888 | 42.701 | 1.00 | 23.86 |
| ATOM | 989  | CG2 | ILE | 128 | 14.272 | 45.120 | 41.577 | 1.00 | 28.95 |
| ATOM | 990  | CD1 | ILE | 128 | 15.824 | 46.391 | 44.013 | 1.00 | 29.89 |
| ATOM | 991  | N   | ASP | 129 | 16.999 | 48.002 | 39.918 | 1.00 | 20.26 |
| ATOM | 992  | CA  | ASP | 129 | 17.861 | 49.124 | 39.882 | 1.00 | 18.53 |
| ATOM | 993  | C   | ASP | 129 | 18.864 | 49.086 | 38.801 | 1.00 | 20.36 |
| ATOM | 994  | O   | ASP | 129 | 19.949 | 49.632 | 38.953 | 1.00 | 24.28 |
| ATOM | 995  | CB  | ASP | 129 | 18.498 | 49.407 | 41.253 | 1.00 | 20.57 |
| ATOM | 996  | CG  | ASP | 129 | 17.545 | 50.077 | 42.226 | 1.00 | 43.70 |
| ATOM | 997  | OD1 | ASP | 129 | 16.653 | 50.842 | 41.883 | 1.00 | 49.42 |
| ATOM | 998  | OD2 | ASP | 129 | 17.770 | 49.740 | 43.475 | 1.00 | 38.07 |
| ATOM | 999  | N   | PHE | 130 | 18.510 | 48.493 | 37.693 | 1.00 | 16.40 |
| ATOM | 1000 | CA  | PHE | 130 | 19.433 | 48.459 | 36.563 | 1.00 | 16.99 |
| ATOM | 1001 | C   | PHE | 130 | 19.330 | 49.732 | 35.576 | 1.00 | 35.37 |
| ATOM | 1002 | O   | PHE | 130 | 18.242 | 50.318 | 35.623 | 1.00 | 27.34 |
| ATOM | 1003 | CB  | PHE | 130 | 19.248 | 47.223 | 35.657 | 1.00 | 18.07 |
| ATOM | 1004 | CG  | PHE | 130 | 19.809 | 45.980 | 36.312 | 1.00 | 19.10 |
| ATOM | 1005 | CD1 | PHE | 130 | 19.021 | 45.210 | 37.171 | 1.00 | 16.15 |
| ATOM | 1006 | CD2 | PHE | 130 | 21.126 | 45.572 | 36.073 | 1.00 | 19.17 |
| ATOM | 1007 | CE1 | PHE | 130 | 19.536 | 44.074 | 37.801 | 1.00 | 23.37 |
| ATOM | 1008 | CE2 | PHE | 130 | 21.665 | 44.445 | 36.703 | 1.00 | 21.11 |
| ATOM | 1009 | CZ  | PHE | 130 | 20.867 | 43.703 | 37.575 | 1.00 | 22.13 |
| ATOM | 1010 | N   | LYS | 131 | 20.464 | 50.169 | 35.218 | 1.00 | 31.09 |
| ATOM | 1011 | CA  | LYS | 131 | 20.477 | 51.371 | 34.400 | 1.00 | 27.52 |
| ATOM | 1012 | C   | LYS | 131 | 20.105 | 51.045 | 32.992 | 1.00 | 25.57 |
| ATOM | 1013 | O   | LYS | 131 | 20.695 | 50.169 | 32.343 | 1.00 | 22.97 |
| ATOM | 1014 | CB  | LYS | 131 | 21.796 | 52.109 | 34.438 | 1.00 | 32.64 |
| ATOM | 1015 | CG  | LYS | 131 | 22.153 | 52.633 | 35.813 | 1.00 | 38.34 |
| ATOM | 1016 | CD  | LYS | 131 | 23.646 | 52.886 | 35.975 | 1.00 | 75.76 |
| ATOM | 1017 | N   | GLU | 132 | 19.116 | 51.751 | 32.509 | 1.00 | 26.88 |
| ATOM | 1018 | CA  | GLU | 132 | 18.623 | 51.484 | 31.189 | 1.00 | 28.42 |
| ATOM | 1019 | C   | GLU | 132 | 19.710 | 51.514 | 30.140 | 1.00 | 36.19 |

**FIG. 5Y**

|      |          |     |     |        |        |        |             |
|------|----------|-----|-----|--------|--------|--------|-------------|
| ATOM | 1020 O   | GLU | 132 | 19.617 | 50.862 | 29.101 | 1.00 39.24  |
| ATOM | 1021 CB  | GLU | 132 | 17.374 | 52.331 | 30.830 | 1.00 29.04  |
| ATOM | 1022 N   | ASP | 133 | 20.752 | 52.254 | 30.438 | 1.00 40.08  |
| ATOM | 1023 CA  | ASP | 133 | 21.883 | 52.442 | 29.525 | 1.00 45.36  |
| ATOM | 1024 C   | ASP | 133 | 23.224 | 51.861 | 30.049 | 1.00 50.61  |
| ATOM | 1025 O   | ASP | 133 | 24.299 | 52.243 | 29.572 | 1.00 52.14  |
| ATOM | 1026 CB  | ASP | 133 | 22.063 | 53.946 | 29.332 | 1.00 50.45  |
| ATOM | 1027 CG  | ASP | 133 | 22.109 | 54.642 | 30.670 | 1.00 87.10  |
| ATOM | 1028 OD1 | ASP | 133 | 21.408 | 54.314 | 31.624 | 1.00 91.27  |
| ATOM | 1029 OD2 | ASP | 133 | 23.047 | 55.552 | 30.739 | 1.00 100.00 |
| ATOM | 1030 N   | GLY | 134 | 23.159 | 50.970 | 31.053 | 1.00 37.06  |
| ATOM | 1031 CA  | GLY | 134 | 24.349 | 50.376 | 31.639 | 1.00 30.22  |
| ATOM | 1032 C   | GLY | 134 | 24.845 | 49.228 | 30.803 | 1.00 23.10  |
| ATOM | 1033 O   | GLY | 134 | 24.360 | 48.990 | 29.685 | 1.00 19.23  |
| ATOM | 1034 N   | ASN | 135 | 25.807 | 48.486 | 31.341 | 1.00 18.66  |
| ATOM | 1035 CA  | ASN | 135 | 26.339 | 47.370 | 30.563 | 1.00 18.03  |
| ATOM | 1036 C   | ASN | 135 | 25.372 | 46.199 | 30.406 | 1.00 15.75  |
| ATOM | 1037 O   | ASN | 135 | 25.485 | 45.430 | 29.461 | 1.00 16.03  |
| ATOM | 1038 CB  | ASN | 135 | 27.665 | 46.883 | 31.139 | 1.00 19.27  |
| ATOM | 1039 CG  | ASN | 135 | 28.743 | 47.943 | 31.108 | 1.00 20.99  |
| ATOM | 1040 OD1 | ASN | 135 | 28.969 | 48.595 | 30.078 | 1.00 25.69  |
| ATOM | 1041 ND2 | ASN | 135 | 29.423 | 48.095 | 32.239 | 1.00 22.57  |
| ATOM | 1042 N   | ILE | 136 | 24.444 | 46.052 | 31.362 | 1.00 18.14  |
| ATOM | 1043 CA  | ILE | 136 | 23.494 | 44.924 | 31.368 | 1.00 19.78  |
| ATOM | 1044 C   | ILE | 136 | 22.331 | 45.086 | 30.384 | 1.00 23.76  |
| ATOM | 1045 O   | ILE | 136 | 22.178 | 44.313 | 29.395 | 1.00 22.53  |
| ATOM | 1046 CB  | ILE | 136 | 23.078 | 44.500 | 32.804 | 1.00 21.24  |
| ATOM | 1047 CG1 | ILE | 136 | 24.230 | 43.728 | 33.423 | 1.00 28.44  |
| ATOM | 1048 CG2 | ILE | 136 | 21.899 | 43.543 | 32.770 | 1.00 22.77  |
| ATOM | 1049 CD1 | ILE | 136 | 25.346 | 44.596 | 33.935 | 1.00 12.39  |
| ATOM | 1050 N   | LEU | 137 | 21.543 | 46.117 | 30.640 | 1.00 18.21  |
| ATOM | 1051 CA  | LEU | 137 | 20.394 | 46.415 | 29.815 | 1.00 23.30  |
| ATOM | 1052 C   | LEU | 137 | 20.828 | 46.875 | 28.470 | 1.00 27.26  |
| ATOM | 1053 O   | LEU | 137 | 20.181 | 46.619 | 27.488 | 1.00 27.00  |
| ATOM | 1054 CB  | LEU | 137 | 19.442 | 47.430 | 30.490 | 1.00 21.74  |
| ATOM | 1055 CG  | LEU | 137 | 18.828 | 46.852 | 31.762 | 1.00 22.56  |
| ATOM | 1056 CD1 | LEU | 137 | 17.856 | 47.837 | 32.415 | 1.00 22.27  |
| ATOM | 1057 CD2 | LEU | 137 | 18.118 | 45.554 | 31.424 | 1.00 37.52  |
| ATOM | 1058 N   | GLY | 138 | 21.979 | 47.527 | 28.432 | 1.00 22.14  |
| ATOM | 1059 CA  | GLY | 138 | 22.510 | 48.033 | 27.187 | 1.00 20.03  |
| ATOM | 1060 C   | GLY | 138 | 23.157 | 46.959 | 26.368 | 1.00 20.16  |

**FIG. 5Z**



|      |          |     |     |        |        |        |            |
|------|----------|-----|-----|--------|--------|--------|------------|
| ATOM | 1061 O   | GLY | 138 | 23.600 | 47.202 | 25.264 | 1.00 22.44 |
| ATOM | 1062 N   | HIS | 139 | 23.246 | 45.756 | 26.903 | 1.00 18.27 |
| ATOM | 1063 CA  | HIS | 139 | 23.859 | 44.655 | 26.148 | 1.00 20.24 |
| ATOM | 1064 C   | HIS | 139 | 25.301 | 44.929 | 25.616 | 1.00 20.13 |
| ATOM | 1065 O   | HIS | 139 | 25.605 | 44.745 | 24.439 | 1.00 17.97 |
| ATOM | 1066 CB  | HIS | 139 | 22.931 | 44.207 | 25.018 | 1.00 22.20 |
| ATOM | 1067 CG  | HIS | 139 | 21.708 | 43.551 | 25.550 | 1.00 25.52 |
| ATOM | 1068 ND1 | HIS | 139 | 21.666 | 42.182 | 25.785 | 1.00 25.67 |
| ATOM | 1069 CD2 | HIS | 139 | 20.525 | 44.092 | 25.927 | 1.00 28.09 |
| ATOM | 1070 CE1 | HIS | 139 | 20.474 | 41.918 | 26.275 | 1.00 27.50 |
| ATOM | 1071 NE2 | HIS | 139 | 19.766 | 43.044 | 26.382 | 1.00 29.53 |
| ATOM | 1072 N   | LYS | 140 | 26.187 | 45.311 | 26.525 | 1.00 23.51 |
| ATOM | 1073 CA  | LYS | 140 | 27.569 | 45.638 | 26.197 | 1.00 25.82 |
| ATOM | 1074 C   | LYS | 140 | 28.600 | 44.537 | 26.560 | 1.00 26.28 |
| ATOM | 1075 O   | LYS | 140 | 29.824 | 44.730 | 26.391 | 1.00 22.29 |
| ATOM | 1076 CB  | LYS | 140 | 27.977 | 46.937 | 26.911 | 1.00 27.56 |
| ATOM | 1077 CG  | LYS | 140 | 27.269 | 48.217 | 26.445 | 1.00 31.19 |
| ATOM | 1078 CD  | LYS | 140 | 27.234 | 49.254 | 27.582 | 1.00 51.32 |
| ATOM | 1079 CE  | LYS | 140 | 26.924 | 50.696 | 27.169 | 1.00 47.92 |
| ATOM | 1080 NZ  | LYS | 140 | 27.112 | 51.663 | 28.284 | 1.00 73.76 |
| ATOM | 1081 N   | LEU | 141 | 28.116 | 43.403 | 27.115 | 1.00 19.33 |
| ATOM | 1082 CA  | LEU | 141 | 28.987 | 42.296 | 27.559 | 1.00 14.32 |
| ATOM | 1083 C   | LEU | 141 | 29.366 | 41.401 | 26.427 | 1.00 20.75 |
| ATOM | 1084 O   | LEU | 141 | 28.526 | 41.087 | 25.620 | 1.00 19.01 |
| ATOM | 1085 CB  | LEU | 141 | 28.313 | 41.488 | 28.676 | 1.00 12.53 |
| ATOM | 1086 CG  | LEU | 141 | 27.979 | 42.352 | 29.875 | 1.00 17.54 |
| ATOM | 1087 CD1 | LEU | 141 | 27.700 | 41.469 | 31.070 | 1.00 24.81 |
| ATOM | 1088 CD2 | LEU | 141 | 29.116 | 43.310 | 30.182 | 1.00 27.50 |
| ATOM | 1089 N   | GLU | 142 | 30.644 | 40.987 | 26.346 | 1.00 14.76 |
| ATOM | 1090 CA  | GLU | 142 | 31.040 | 40.059 | 25.311 | 1.00 13.43 |
| ATOM | 1091 C   | GLU | 142 | 30.462 | 38.691 | 25.641 | 1.00 15.69 |
| ATOM | 1092 O   | GLU | 142 | 30.175 | 38.393 | 26.787 | 1.00 16.43 |
| ATOM | 1093 CB  | GLU | 142 | 32.558 | 39.866 | 25.204 | 1.00 14.73 |
| ATOM | 1094 CG  | GLU | 142 | 33.290 | 41.077 | 24.624 | 1.00 29.30 |
| ATOM | 1095 CD  | GLU | 142 | 34.787 | 41.003 | 24.825 | 1.00 56.32 |
| ATOM | 1096 OE1 | GLU | 142 | 35.340 | 40.098 | 25.420 | 1.00 31.70 |
| ATOM | 1097 OE2 | GLU | 142 | 35.430 | 42.015 | 24.321 | 1.00 34.10 |
| ATOM | 1098 N   | TYR | 143 | 30.365 | 37.873 | 24.632 | 1.00 16.30 |
| ATOM | 1099 CA  | TYR | 143 | 29.837 | 36.542 | 24.764 | 1.00 20.04 |
| ATOM | 1100 C   | TYR | 143 | 30.925 | 35.559 | 25.049 | 1.00 12.46 |
| ATOM | 1101 O   | TYR | 143 | 31.327 | 34.792 | 24.193 | 1.00 16.99 |

**FIG. 5AA**

|      |             |     |        |        |        |      |       |
|------|-------------|-----|--------|--------|--------|------|-------|
| ATOM | 1102 CB TYR | 143 | 29.035 | 36.118 | 23.498 | 1.00 | 20.96 |
| ATOM | 1103 CG TYR | 143 | 28.187 | 34.857 | 23.674 | 1.00 | 16.12 |
| ATOM | 1104 CD1TYR | 143 | 27.040 | 34.859 | 24.472 | 1.00 | 18.24 |
| ATOM | 1105 CD2TYR | 143 | 28.512 | 33.684 | 22.986 | 1.00 | 12.87 |
| ATOM | 1106 CE1TYR | 143 | 26.257 | 33.708 | 24.615 | 1.00 | 17.91 |
| ATOM | 1107 CE2TYR | 143 | 27.735 | 32.530 | 23.104 | 1.00 | 16.58 |
| ATOM | 1108 CZ TYR | 143 | 26.603 | 32.551 | 23.914 | 1.00 | 17.35 |
| ATOM | 1109 OH TYR | 143 | 25.861 | 31.432 | 24.035 | 1.00 | 23.40 |
| ATOM | 1110 N ASN  | 144 | 31.392 | 35.597 | 26.251 | 1.00 | 12.40 |
| ATOM | 1111 CA ASN | 144 | 32.428 | 34.703 | 26.689 | 1.00 | 12.05 |
| ATOM | 1112 C ASN  | 144 | 32.433 | 34.675 | 28.193 | 1.00 | 15.75 |
| ATOM | 1113 O ASN  | 144 | 31.637 | 35.369 | 28.837 | 1.00 | 14.58 |
| ATOM | 1114 CB ASN | 144 | 33.823 | 35.038 | 26.068 | 1.00 | 18.45 |
| ATOM | 1115 CG ASN | 144 | 34.310 | 36.445 | 26.374 | 1.00 | 18.98 |
| ATOM | 1116 OD1ASN | 144 | 34.150 | 36.951 | 27.488 | 1.00 | 20.34 |
| ATOM | 1117 ND2ASN | 144 | 34.891 | 37.085 | 25.382 | 1.00 | 23.02 |
| ATOM | 1118 N TYR  | 145 | 33.311 | 33.876 | 28.773 | 1.00 | 12.16 |
| ATOM | 1119 CA TYR | 145 | 33.343 | 33.765 | 30.195 | 1.00 | 10.63 |
| ATOM | 1120 C TYR  | 145 | 34.765 | 33.458 | 30.730 | 1.00 | 14.58 |
| ATOM | 1121 O TYR  | 145 | 35.510 | 32.751 | 30.090 | 1.00 | 18.83 |
| ATOM | 1122 CB TYR | 145 | 32.404 | 32.627 | 30.571 | 1.00 | 9.76  |
| ATOM | 1123 CG TYR | 145 | 31.698 | 32.916 | 31.826 | 1.00 | 11.86 |
| ATOM | 1124 CD1TYR | 145 | 30.515 | 33.658 | 31.808 | 1.00 | 9.04  |
| ATOM | 1125 CD2TYR | 145 | 32.188 | 32.419 | 33.030 | 1.00 | 10.07 |
| ATOM | 1126 CE1TYR | 145 | 29.860 | 33.948 | 32.999 | 1.00 | 8.36  |
| ATOM | 1127 CE2TYR | 145 | 31.544 | 32.707 | 34.235 | 1.00 | 15.32 |
| ATOM | 1128 CZ TYR | 145 | 30.375 | 33.469 | 34.206 | 1.00 | 11.69 |
| ATOM | 1129 OH TYR | 145 | 29.730 | 33.735 | 35.376 | 1.00 | 15.23 |
| ATOM | 1130 N ASN  | 146 | 35.086 | 33.931 | 31.933 | 1.00 | 15.36 |
| ATOM | 1131 CA ASN | 146 | 36.415 | 33.737 | 32.560 | 1.00 | 17.00 |
| ATOM | 1132 C ASN  | 146 | 36.426 | 32.618 | 33.589 | 1.00 | 19.68 |
| ATOM | 1133 O ASN  | 146 | 35.395 | 32.043 | 33.848 | 1.00 | 14.71 |
| ATOM | 1134 CB ASN | 146 | 36.844 | 35.062 | 33.235 | 1.00 | 11.89 |
| ATOM | 1135 CG ASN | 146 | 37.013 | 36.147 | 32.215 | 1.00 | 35.45 |
| ATOM | 1136 OD1ASN | 146 | 37.533 | 35.890 | 31.105 | 1.00 | 31.63 |
| ATOM | 1137 ND2ASN | 146 | 36.547 | 37.349 | 32.553 | 1.00 | 19.74 |
| ATOM | 1138 N SER  | 147 | 37.630 | 32.338 | 34.201 | 1.00 | 12.09 |
| ATOM | 1139 CA SER | 147 | 37.804 | 31.320 | 35.266 | 1.00 | 8.55  |
| ATOM | 1140 C SER  | 147 | 37.769 | 31.999 | 36.575 | 1.00 | 11.70 |
| ATOM | 1141 O SER  | 147 | 38.219 | 33.125 | 36.671 | 1.00 | 16.56 |
| ATOM | 1142 CB SER | 147 | 39.148 | 30.540 | 35.129 | 1.00 | 9.87  |
| ATOM | 1143 OG SER | 147 | 39.212 | 29.980 | 33.828 | 1.00 | 33.20 |

**FIG. 5AB**

|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1144 | N   | HIS | 148 | 37.195 | 31.365 | 37.583 | 1.00 | 5.53  |
| ATOM | 1145 | CA  | HIS | 148 | 37.090 | 31.998 | 38.850 | 1.00 | 8.06  |
| ATOM | 1146 | C   | HIS | 148 | 37.346 | 31.038 | 39.949 | 1.00 | 11.30 |
| ATOM | 1147 | O   | HIS | 148 | 37.328 | 29.844 | 39.754 | 1.00 | 16.87 |
| ATOM | 1148 | CB  | HIS | 148 | 35.648 | 32.608 | 39.067 | 1.00 | 11.29 |
| ATOM | 1149 | CG  | HIS | 148 | 35.215 | 33.554 | 37.972 | 1.00 | 10.84 |
| ATOM | 1150 | ND1 | HIS | 148 | 34.548 | 33.121 | 36.836 | 1.00 | 12.77 |
| ATOM | 1151 | CD2 | HIS | 148 | 35.403 | 34.887 | 37.851 | 1.00 | 8.82  |
| ATOM | 1152 | CE1 | HIS | 148 | 34.389 | 34.178 | 36.060 | 1.00 | 8.84  |
| ATOM | 1153 | NE2 | HIS | 148 | 34.882 | 35.242 | 36.647 | 1.00 | 8.82  |
| ATOM | 1154 | N   | ASN | 149 | 37.534 | 31.579 | 41.125 | 1.00 | 10.80 |
| ATOM | 1155 | CA  | ASN | 149 | 37.626 | 30.805 | 42.345 | 1.00 | 13.35 |
| ATOM | 1156 | C   | ASN | 149 | 36.409 | 31.157 | 43.205 | 1.00 | 14.47 |
| ATOM | 1157 | O   | ASN | 149 | 36.099 | 32.320 | 43.387 | 1.00 | 18.17 |
| ATOM | 1158 | CB  | ASN | 149 | 38.890 | 31.093 | 43.184 | 1.00 | 12.67 |
| ATOM | 1159 | CG  | ASN | 149 | 40.148 | 30.822 | 42.424 | 1.00 | 20.21 |
| ATOM | 1160 | OD1 | ASN | 149 | 40.993 | 31.713 | 42.281 | 1.00 | 56.34 |
| ATOM | 1161 | ND2 | ASN | 149 | 40.210 | 29.641 | 41.818 | 1.00 | 16.44 |
| ATOM | 1162 | N   | VAL | 150 | 35.773 | 30.144 | 43.741 | 1.00 | 14.65 |
| ATOM | 1163 | CA  | VAL | 150 | 34.588 | 30.262 | 44.552 | 1.00 | 12.92 |
| ATOM | 1164 | C   | VAL | 150 | 34.910 | 29.806 | 45.943 | 1.00 | 16.30 |
| ATOM | 1165 | O   | VAL | 150 | 35.257 | 28.665 | 46.147 | 1.00 | 17.83 |
| ATOM | 1166 | CB  | VAL | 150 | 33.482 | 29.382 | 43.914 | 1.00 | 15.22 |
| ATOM | 1167 | CG1 | VAL | 150 | 32.252 | 29.297 | 44.765 | 1.00 | 14.09 |
| ATOM | 1168 | CG2 | VAL | 150 | 33.172 | 29.791 | 42.464 | 1.00 | 10.94 |
| ATOM | 1169 | N   | TYR | 151 | 34.796 | 30.716 | 46.900 | 1.00 | 17.64 |
| ATOM | 1170 | CA  | TYR | 151 | 35.139 | 30.440 | 48.275 | 1.00 | 18.31 |
| ATOM | 1171 | C   | TYR | 151 | 34.003 | 29.917 | 49.117 | 1.00 | 24.35 |
| ATOM | 1172 | O   | TYR | 151 | 32.963 | 30.536 | 49.239 | 1.00 | 20.83 |
| ATOM | 1173 | CB  | TYR | 151 | 35.793 | 31.681 | 48.920 | 1.00 | 20.15 |
| ATOM | 1174 | CG  | TYR | 151 | 37.025 | 32.033 | 48.141 | 1.00 | 25.86 |
| ATOM | 1175 | CD1 | TYR | 151 | 37.003 | 32.989 | 47.127 | 1.00 | 26.00 |
| ATOM | 1176 | CD2 | TYR | 151 | 38.200 | 31.315 | 48.355 | 1.00 | 28.66 |
| ATOM | 1177 | CE1 | TYR | 151 | 38.151 | 33.234 | 46.369 | 1.00 | 33.73 |
| ATOM | 1178 | CE2 | TYR | 151 | 39.360 | 31.550 | 47.619 | 1.00 | 29.01 |
| ATOM | 1179 | CZ  | TYR | 151 | 39.325 | 32.512 | 46.618 | 1.00 | 29.55 |
| ATOM | 1180 | OH  | TYR | 151 | 40.449 | 32.737 | 45.877 | 1.00 | 38.69 |
| ATOM | 1181 | N   | ILE | 152 | 34.250 | 28.791 | 49.753 | 1.00 | 17.71 |
| ATOM | 1182 | CA  | ILE | 152 | 33.255 | 28.159 | 50.572 | 1.00 | 14.12 |
| ATOM | 1183 | C   | ILE | 152 | 33.619 | 28.056 | 52.000 | 1.00 | 18.51 |
| ATOM | 1184 | O   | ILE | 152 | 34.728 | 27.703 | 52.336 | 1.00 | 22.05 |

**FIG. 5AC**

|      |          |     |     |        |        |        |             |
|------|----------|-----|-----|--------|--------|--------|-------------|
| ATOM | 1185 CB  | ILE | 152 | 32.979 | 26.776 | 50.060 | 1.00 16.66  |
| ATOM | 1186 CG1 | ILE | 152 | 32.431 | 26.875 | 48.638 | 1.00 11.30  |
| ATOM | 1187 CG2 | ILE | 152 | 32.017 | 26.078 | 51.021 | 1.00 17.96  |
| ATOM | 1188 CD1 | ILE | 152 | 32.377 | 25.559 | 47.949 | 1.00 13.48  |
| ATOM | 1189 N   | MSE | 153 | 32.623 | 28.278 | 52.841 | 1.00 17.41  |
| ATOM | 1190 AC  | MSE | 153 | 32.789 | 28.162 | 54.269 | 1.00 22.61  |
| ATOM | 1191 C   | MSE | 153 | 31.534 | 27.648 | 54.916 | 1.00 27.31  |
| ATOM | 1192 O   | MSE | 153 | 30.433 | 27.831 | 54.396 | 1.00 20.50  |
| ATOM | 1193 CB  | MSE | 153 | 33.145 | 29.490 | 54.855 | 1.00 19.11  |
| ATOM | 1194 CG  | MSE | 153 | 34.010 | 30.302 | 53.957 | 1.00 100.00 |
| ATOM | 1195 SE  | MSE | 153 | 34.060 | 32.117 | 54.524 | 1.00 100.00 |
| ATOM | 1196 CE  | MSE | 153 | 33.463 | 31.798 | 56.330 | 1.00 30.27  |
| ATOM | 1197 N   | ALA | 154 | 31.733 | 26.983 | 56.053 | 1.00 22.29  |
| ATOM | 1198 CA  | ALA | 154 | 30.669 | 26.389 | 56.796 | 1.00 22.66  |
| ATOM | 1199 C   | ALA | 154 | 29.820 | 27.401 | 57.552 | 1.00 29.00  |
| ATOM | 1200 O   | ALA | 154 | 30.274 | 28.457 | 57.960 | 1.00 27.02  |
| ATOM | 1201 CB  | ALA | 154 | 31.224 | 25.336 | 57.744 | 1.00 19.78  |
| ATOM | 1202 N   | ASP | 155 | 28.566 | 27.063 | 57.726 | 1.00 29.48  |
| ATOM | 1203 CA  | ASP | 155 | 27.669 | 27.887 | 58.484 | 1.00 32.18  |
| ATOM | 1204 C   | ASP | 155 | 26.976 | 27.019 | 59.511 | 1.00 44.51  |
| ATOM | 1205 O   | ASP | 155 | 25.898 | 26.492 | 59.274 | 1.00 39.56  |
| ATOM | 1206 CB  | ASP | 155 | 26.659 | 28.617 | 57.597 | 1.00 31.70  |
| ATOM | 1207 CG  | ASP | 155 | 26.140 | 29.851 | 58.247 | 1.00 49.89  |
| ATOM | 1208 OD1 | ASP | 155 | 26.595 | 30.297 | 59.277 | 1.00 46.67  |
| ATOM | 1209 OD2 | ASP | 155 | 25.187 | 30.422 | 57.565 | 1.00 76.07  |
| ATOM | 1210 N   | LYS | 156 | 27.646 | 26.816 | 60.629 | 1.00 46.37  |
| ATOM | 1211 CA  | LYS | 156 | 27.116 | 25.954 | 61.654 | 1.00 53.23  |
| ATOM | 1212 C   | LYS | 156 | 25.750 | 26.369 | 62.224 | 1.00 65.62  |
| ATOM | 1213 O   | LYS | 156 | 25.012 | 25.520 | 62.703 | 1.00 65.54  |
| ATOM | 1214 CB  | LYS | 156 | 28.147 | 25.612 | 62.725 | 1.00 59.51  |
| ATOM | 1215 N   | GLN | 157 | 25.398 | 27.655 | 62.138 | 1.00 68.32  |
| ATOM | 1216 CA  | GLN | 157 | 24.119 | 28.135 | 62.670 | 1.00 73.00  |
| ATOM | 1217 C   | GLN | 157 | 22.891 | 27.767 | 61.817 | 1.00 87.53  |
| ATOM | 1218 O   | GLN | 157 | 21.778 | 27.547 | 62.325 | 1.00 96.16  |
| ATOM | 1219 N   | LYS | 158 | 23.095 | 27.725 | 60.506 | 1.00 72.49  |
| ATOM | 1220 CA  | LYS | 158 | 22.040 | 27.386 | 59.593 | 1.00 66.19  |
| ATOM | 1221 C   | LYS | 158 | 22.235 | 25.985 | 59.040 | 1.00 58.21  |
| ATOM | 1222 O   | LYS | 158 | 21.447 | 25.524 | 58.226 | 1.00 59.85  |
| ATOM | 1223 N   | ASN | 159 | 23.303 | 25.294 | 59.502 | 1.00 40.00  |
| ATOM | 1224 CA  | ASN | 159 | 23.582 | 23.944 | 59.012 | 1.00 36.67  |
| ATOM | 1225 C   | ASN | 159 | 23.755 | 24.002 | 57.500 | 1.00 34.11  |

**FIG. 5AD**

|      |      |     |     |     |        |        |        |      |        |
|------|------|-----|-----|-----|--------|--------|--------|------|--------|
| ATOM | 1226 | CO  | ASN | 159 | 23.223 | 23.167 | 56.754 | 1.00 | 31.69  |
| ATOM | 1227 | CB  | ASN | 159 | 22.431 | 22.952 | 59.367 | 1.00 | 46.42  |
| ATOM | 1228 | CG  | ASN | 159 | 22.842 | 21.485 | 59.428 | 1.00 | 80.46  |
| ATOM | 1229 | OD1 | ASN | 159 | 23.850 | 21.121 | 60.054 | 1.00 | 100.00 |
| ATOM | 1230 | ND2 | ASN | 159 | 22.003 | 20.620 | 58.854 | 1.00 | 58.09  |
| ATOM | 1231 | N   | GLY | 160 | 24.474 | 25.044 | 57.062 | 1.00 | 22.34  |
| ATOM | 1232 | CA  | GLY | 160 | 24.686 | 25.247 | 55.663 | 1.00 | 17.58  |
| ATOM | 1233 | C   | GLY | 160 | 26.055 | 25.791 | 55.433 | 1.00 | 26.75  |
| ATOM | 1234 | O   | GLY | 160 | 26.960 | 25.664 | 56.271 | 1.00 | 25.57  |
| ATOM | 1235 | N   | ILE | 161 | 26.200 | 26.395 | 54.277 | 1.00 | 23.28  |
| ATOM | 1236 | CA  | ILE | 161 | 27.442 | 26.975 | 53.909 | 1.00 | 16.45  |
| ATOM | 1237 | C   | ILE | 161 | 27.200 | 28.354 | 53.395 | 1.00 | 15.77  |
| ATOM | 1238 | O   | ILE | 161 | 26.118 | 28.680 | 52.962 | 1.00 | 15.95  |
| ATOM | 1239 | CB  | ILE | 161 | 28.129 | 26.117 | 52.864 | 1.00 | 19.27  |
| ATOM | 1240 | CG1 | ILE | 161 | 27.237 | 26.016 | 51.619 | 1.00 | 18.53  |
| ATOM | 1241 | CG2 | ILE | 161 | 28.351 | 24.735 | 53.445 | 1.00 | 21.96  |
| ATOM | 1242 | CD1 | ILE | 161 | 28.009 | 25.614 | 50.350 | 1.00 | 14.44  |
| ATOM | 1243 | N   | LYS | 162 | 28.226 | 29.169 | 53.471 | 1.00 | 17.86  |
| ATOM | 1244 | CA  | LYS | 162 | 28.187 | 30.508 | 52.948 | 1.00 | 14.42  |
| ATOM | 1245 | C   | LYS | 162 | 29.216 | 30.524 | 51.857 | 1.00 | 17.73  |
| ATOM | 1246 | O   | LYS | 162 | 30.249 | 29.875 | 51.991 | 1.00 | 19.16  |
| ATOM | 1247 | CB  | LYS | 162 | 28.480 | 31.540 | 54.055 | 1.00 | 18.15  |
| ATOM | 1248 | CG  | LYS | 162 | 27.221 | 31.963 | 54.796 | 1.00 | 42.08  |
| ATOM | 1249 | CD  | LYS | 162 | 27.493 | 32.787 | 56.039 | 1.00 | 70.42  |
| ATOM | 1250 | N   | VAL | 163 | 28.911 | 31.176 | 50.759 | 1.00 | 13.74  |
| ATOM | 1251 | CA  | VAL | 163 | 29.798 | 31.201 | 49.629 | 1.00 | 11.95  |
| ATOM | 1252 | C   | VAL | 163 | 29.928 | 32.610 | 49.103 | 1.00 | 19.30  |
| ATOM | 1253 | O   | VAL | 163 | 28.944 | 33.318 | 48.983 | 1.00 | 19.84  |
| ATOM | 1254 | CB  | VAL | 163 | 29.249 | 30.268 | 48.532 | 1.00 | 15.89  |
| ATOM | 1255 | CG1 | VAL | 163 | 30.105 | 30.277 | 47.261 | 1.00 | 12.09  |
| ATOM | 1256 | CG2 | VAL | 163 | 29.029 | 28.852 | 49.077 | 1.00 | 15.86  |
| ATOM | 1257 | N   | ASN | 164 | 31.146 | 32.999 | 48.733 | 1.00 | 14.03  |
| ATOM | 1258 | CA  | ASN | 164 | 31.382 | 34.310 | 48.195 | 1.00 | 15.58  |
| ATOM | 1259 | C   | ASN | 164 | 32.396 | 34.271 | 47.050 | 1.00 | 20.08  |
| ATOM | 1260 | O   | ASN | 164 | 33.268 | 33.386 | 46.988 | 1.00 | 23.49  |
| ATOM | 1261 | CB  | ASN | 164 | 31.732 | 35.325 | 49.308 | 1.00 | 20.52  |
| ATOM | 1262 | CG  | ASN | 164 | 33.196 | 35.697 | 49.330 | 1.00 | 89.21  |
| ATOM | 1263 | OD1 | ASN | 164 | 34.020 | 34.987 | 49.929 | 1.00 | 100.00 |
| ATOM | 1264 | ND2 | ASN | 164 | 33.515 | 36.831 | 48.700 | 1.00 | 91.46  |
| ATOM | 1265 | N   | PHE | 165 | 32.244 | 35.207 | 46.109 | 1.00 | 17.37  |
| ATOM | 1266 | CA  | PHE | 165 | 33.133 | 35.301 | 44.953 | 1.00 | 10.86  |

**FIG. 5AE**

|      |          |     |     |        |        |        |            |
|------|----------|-----|-----|--------|--------|--------|------------|
| ATOM | 1267 C   | PHE | 165 | 32.751 | 36.445 | 44.071 | 1.00 15.53 |
| ATOM | 1268 O   | PHE | 165 | 31.686 | 37.020 | 44.251 | 1.00 17.16 |
| ATOM | 1269 CB  | PHE | 165 | 33.207 | 33.960 | 44.187 | 1.00 12.86 |
| ATOM | 1270 CG  | PHE | 165 | 31.862 | 33.486 | 43.622 | 1.00 14.35 |
| ATOM | 1271 CD1 | PHE | 165 | 31.510 | 33.749 | 42.293 | 1.00 14.61 |
| ATOM | 1272 CD2 | PHE | 165 | 30.978 | 32.757 | 44.413 | 1.00 13.56 |
| ATOM | 1273 CE1 | PHE | 165 | 30.300 | 33.297 | 41.759 | 1.00 22.67 |
| ATOM | 1274 CE2 | PHE | 165 | 29.774 | 32.282 | 43.893 | 1.00 15.78 |
| ATOM | 1275 CZ  | PHE | 165 | 29.426 | 32.572 | 42.573 | 1.00 16.20 |
| ATOM | 1276 N   | LYS | 166 | 33.641 | 36.799 | 43.132 | 1.00 10.79 |
| ATOM | 1277 CA  | LYS | 166 | 33.417 | 37.864 | 42.162 | 1.00 10.74 |
| ATOM | 1278 C   | LYS | 166 | 33.603 | 37.344 | 40.774 | 1.00 15.95 |
| ATOM | 1279 O   | LYS | 166 | 34.602 | 36.727 | 40.470 | 1.00 22.80 |
| ATOM | 1280 CB  | LYS | 166 | 34.387 | 39.055 | 42.249 | 1.00 16.61 |
| ATOM | 1281 CG  | LYS | 166 | 34.573 | 39.688 | 43.573 | 1.00 18.11 |
| ATOM | 1282 CD  | LYS | 166 | 35.540 | 40.875 | 43.454 | 1.00 32.56 |
| ATOM | 1283 CE  | LYS | 166 | 35.272 | 41.966 | 44.476 | 1.00 48.19 |
| ATOM | 1284 NZ  | LYS | 166 | 34.823 | 41.435 | 45.782 | 1.00 85.81 |
| ATOM | 1285 N   | ILE | 167 | 32.703 | 37.704 | 39.911 | 1.00 9.75  |
| ATOM | 1286 CA  | ILE | 167 | 32.768 | 37.340 | 38.558 | 1.00 9.35  |
| ATOM | 1287 C   | ILE | 167 | 33.203 | 38.542 | 37.823 | 1.00 14.36 |
| ATOM | 1288 O   | ILE | 167 | 32.811 | 39.640 | 38.170 | 1.00 16.22 |
| ATOM | 1289 CB  | ILE | 167 | 31.379 | 36.929 | 38.005 | 1.00 13.16 |
| ATOM | 1290 CG1 | ILE | 167 | 30.909 | 35.624 | 38.669 | 1.00 13.02 |
| ATOM | 1291 CG2 | ILE | 167 | 31.423 | 36.786 | 36.472 | 1.00 7.91  |
| ATOM | 1292 CD1 | ILE | 167 | 31.773 | 34.415 | 38.344 | 1.00 19.57 |
| ATOM | 1293 N   | ARG | 168 | 34.005 | 38.299 | 36.815 | 1.00 12.19 |
| ATOM | 1294 CA  | ARG | 168 | 34.500 | 39.308 | 35.945 | 1.00 15.07 |
| ATOM | 1295 C   | ARG | 168 | 33.948 | 39.122 | 34.528 | 1.00 16.64 |
| ATOM | 1296 O   | ARG | 168 | 34.278 | 38.156 | 33.836 | 1.00 17.70 |
| ATOM | 1297 CB  | ARG | 168 | 36.024 | 39.287 | 35.944 | 1.00 16.54 |
| ATOM | 1298 CG  | ARG | 168 | 36.580 | 39.632 | 37.321 | 1.00 25.54 |
| ATOM | 1299 CD  | ARG | 168 | 37.894 | 38.910 | 37.601 | 1.00 63.52 |
| ATOM | 1300 NE  | ARG | 168 | 38.380 | 38.191 | 36.416 | 1.00 73.52 |
| ATOM | 1301 CZ  | ARG | 168 | 38.764 | 36.926 | 36.416 | 1.00 67.92 |
| ATOM | 1302 NH1 | ARG | 168 | 38.795 | 36.192 | 37.527 | 1.00 57.44 |
| ATOM | 1303 NH2 | ARG | 168 | 39.192 | 36.375 | 35.271 | 1.00 59.15 |
| ATOM | 1304 N   | HIS | 169 | 33.090 | 40.064 | 34.098 | 1.00 14.88 |
| ATOM | 1305 CA  | HIS | 169 | 32.505 | 40.025 | 32.758 | 1.00 13.24 |
| ATOM | 1306 C   | HIS | 169 | 33.214 | 41.001 | 31.839 | 1.00 12.64 |
| ATOM | 1307 O   | HIS | 169 | 33.306 | 42.203 | 32.121 | 1.00 14.99 |

**FIG. 5AF**

|      |      |     |     |     |        |        |        |      |        |
|------|------|-----|-----|-----|--------|--------|--------|------|--------|
| ATOM | 1308 | CB  | HIS | 169 | 30.970 | 40.374 | 32.760 | 1.00 | 10.46  |
| ATOM | 1309 | CG  | HIS | 169 | 30.097 | 39.474 | 33.573 | 1.00 | 6.54   |
| ATOM | 1310 | ND1 | HIS | 169 | 29.724 | 38.246 | 33.111 | 1.00 | 12.63  |
| ATOM | 1311 | CD2 | HIS | 169 | 29.474 | 39.695 | 34.764 | 1.00 | 10.21  |
| ATOM | 1312 | CE1 | HIS | 169 | 28.892 | 37.718 | 34.031 | 1.00 | 10.53  |
| ATOM | 1313 | NE2 | HIS | 169 | 28.734 | 38.566 | 35.063 | 1.00 | 11.84  |
| ATOM | 1314 | N   | ASN | 170 | 33.691 | 40.513 | 30.737 | 1.00 | 10.66  |
| ATOM | 1315 | CA  | ASN | 170 | 34.349 | 41.368 | 29.812 | 1.00 | 15.87  |
| ATOM | 1316 | C   | ASN | 170 | 33.356 | 42.224 | 29.067 | 1.00 | 25.06  |
| ATOM | 1317 | O   | ASN | 170 | 32.386 | 41.701 | 28.537 | 1.00 | 16.60  |
| ATOM | 1318 | CB  | ASN | 170 | 35.110 | 40.550 | 28.755 | 1.00 | 19.60  |
| ATOM | 1319 | CG  | ASN | 170 | 36.245 | 39.717 | 29.312 | 1.00 | 18.70  |
| ATOM | 1320 | OD1 | ASN | 170 | 36.702 | 38.752 | 28.684 | 1.00 | 48.29  |
| ATOM | 1321 | ND2 | ASN | 170 | 36.695 | 40.073 | 30.480 | 1.00 | 19.13  |
| ATOM | 1322 | N   | ILE | 171 | 33.662 | 43.527 | 28.947 | 1.00 | 18.75  |
| ATOM | 1323 | CA  | ILE | 171 | 32.848 | 44.460 | 28.168 | 1.00 | 16.74  |
| ATOM | 1324 | C   | ILE | 171 | 33.459 | 44.638 | 26.791 | 1.00 | 19.51  |
| ATOM | 1325 | O   | ILE | 171 | 34.643 | 44.596 | 26.642 | 1.00 | 21.06  |
| ATOM | 1326 | CB  | ILE | 171 | 32.713 | 45.804 | 28.842 | 1.00 | 20.46  |
| ATOM | 1327 | CG1 | ILE | 171 | 32.089 | 45.617 | 30.193 | 1.00 | 24.79  |
| ATOM | 1328 | CG2 | ILE | 171 | 31.852 | 46.727 | 27.997 | 1.00 | 19.03  |
| ATOM | 1329 | CD1 | ILE | 171 | 32.630 | 46.599 | 31.229 | 1.00 | 41.65  |
| ATOM | 1330 | N   | GLU | 172 | 32.632 | 44.818 | 25.804 | 1.00 | 16.54  |
| ATOM | 1331 | CA  | GLU | 172 | 33.034 | 44.933 | 24.420 | 1.00 | 17.00  |
| ATOM | 1332 | C   | GLU | 172 | 34.110 | 45.967 | 24.147 | 1.00 | 26.80  |
| ATOM | 1333 | O   | GLU | 172 | 34.776 | 45.898 | 23.125 | 1.00 | 29.20  |
| ATOM | 1334 | CB  | GLU | 172 | 31.813 | 45.165 | 23.509 | 1.00 | 22.46  |
| ATOM | 1335 | CG  | GLU | 172 | 31.122 | 46.531 | 23.786 | 1.00 | 58.53  |
| ATOM | 1336 | CD  | GLU | 172 | 29.871 | 46.783 | 22.933 | 1.00 | 100.00 |
| ATOM | 1337 | OE1 | GLU | 172 | 29.415 | 45.970 | 22.156 | 1.00 | 100.00 |
| ATOM | 1338 | OE2 | GLU | 172 | 29.370 | 47.982 | 23.149 | 1.00 | 100.00 |
| ATOM | 1339 | N   | ASP | 173 | 34.277 | 46.934 | 25.034 | 1.00 | 24.41  |
| ATOM | 1340 | CA  | ASP | 173 | 35.292 | 47.978 | 24.852 | 1.00 | 25.03  |
| ATOM | 1341 | C   | ASP | 173 | 36.651 | 47.624 | 25.455 | 1.00 | 33.40  |
| ATOM | 1342 | O   | ASP | 173 | 37.561 | 48.451 | 25.518 | 1.00 | 30.42  |
| ATOM | 1343 | CB  | ASP | 173 | 34.822 | 49.319 | 25.401 | 1.00 | 23.30  |
| ATOM | 1344 | CG  | ASP | 173 | 34.743 | 49.358 | 26.912 | 1.00 | 32.47  |
| ATOM | 1345 | OD1 | ASP | 173 | 34.406 | 50.355 | 27.513 | 1.00 | 37.58  |
| ATOM | 1346 | OD2 | ASP | 173 | 34.949 | 48.196 | 27.504 | 1.00 | 49.22  |
| ATOM | 1347 | N   | GLY | 174 | 36.766 | 46.410 | 25.956 | 1.00 | 23.87  |
| ATOM | 1348 | CA  | GLY | 174 | 38.019 | 45.994 | 26.537 | 1.00 | 21.30  |

**FIG. 5AG**

|      |          |     |     |        |        |        |            |
|------|----------|-----|-----|--------|--------|--------|------------|
| ATOM | 1349 C   | GLY | 174 | 38.012 | 46.090 | 28.044 | 1.00 19.99 |
| ATOM | 1350 O   | GLY | 174 | 38.927 | 45.585 | 28.709 | 1.00 20.45 |
| ATOM | 1351 N   | SER | 175 | 36.972 | 46.767 | 28.598 | 1.00 13.88 |
| ATOM | 1352 CA  | SER | 175 | 36.898 | 46.931 | 30.034 | 1.00 8.70  |
| ATOM | 1353 C   | SER | 175 | 36.296 | 45.728 | 30.765 | 1.00 17.30 |
| ATOM | 1354 O   | SER | 175 | 36.136 | 44.655 | 30.175 | 1.00 18.77 |
| ATOM | 1355 CB  | SER | 175 | 36.288 | 48.235 | 30.450 | 1.00 14.07 |
| ATOM | 1356 OG  | SER | 175 | 36.360 | 48.316 | 31.865 | 1.00 24.79 |
| ATOM | 1357 N   | VAL | 176 | 35.963 | 45.912 | 32.051 | 1.00 13.74 |
| ATOM | 1358 CA  | VAL | 176 | 35.415 | 44.826 | 32.864 | 1.00 16.46 |
| ATOM | 1359 C   | VAL | 176 | 34.191 | 45.204 | 33.703 | 1.00 22.46 |
| ATOM | 1360 O   | VAL | 176 | 34.159 | 46.254 | 34.334 | 1.00 21.31 |
| ATOM | 1361 CB  | VAL | 176 | 36.477 | 44.285 | 33.818 | 1.00 24.43 |
| ATOM | 1362 CG1 | VAL | 176 | 35.847 | 43.344 | 34.827 | 1.00 27.45 |
| ATOM | 1363 CG2 | VAL | 176 | 37.532 | 43.536 | 33.035 | 1.00 25.65 |
| ATOM | 1364 N   | GLN | 177 | 33.234 | 44.269 | 33.787 | 1.00 15.47 |
| ATOM | 1365 CA  | GLN | 177 | 32.048 | 44.430 | 34.647 | 1.00 15.40 |
| ATOM | 1366 C   | GLN | 177 | 32.102 | 43.457 | 35.813 | 1.00 10.60 |
| ATOM | 1367 O   | GLN | 177 | 32.027 | 42.243 | 35.634 | 1.00 13.65 |
| ATOM | 1368 CB  | GLN | 177 | 30.709 | 44.283 | 33.872 | 1.00 15.57 |
| ATOM | 1369 CG  | GLN | 177 | 29.468 | 44.294 | 34.828 | 1.00 19.13 |
| ATOM | 1370 CD  | GLN | 177 | 29.108 | 45.678 | 35.361 | 1.00 14.91 |
| ATOM | 1371 OE1 | GLN | 177 | 28.759 | 46.588 | 34.574 | 1.00 20.17 |
| ATOM | 1372 NE2 | GLN | 177 | 29.128 | 45.821 | 36.690 | 1.00 17.28 |
| ATOM | 1373 N   | LEU | 178 | 32.227 | 43.993 | 37.018 | 1.00 8.17  |
| ATOM | 1374 CA  | LEU | 178 | 32.313 | 43.180 | 38.181 | 1.00 16.66 |
| ATOM | 1375 C   | LEU | 178 | 30.954 | 42.786 | 38.712 | 1.00 20.93 |
| ATOM | 1376 O   | LEU | 178 | 30.033 | 43.608 | 38.753 | 1.00 14.66 |
| ATOM | 1377 CB  | LEU | 178 | 33.089 | 43.896 | 39.293 | 1.00 20.63 |
| ATOM | 1378 CG  | LEU | 178 | 34.286 | 43.110 | 39.815 | 1.00 39.28 |
| ATOM | 1379 CD1 | LEU | 178 | 33.831 | 42.087 | 40.852 | 1.00 45.14 |
| ATOM | 1380 CD2 | LEU | 178 | 35.018 | 42.426 | 38.648 | 1.00 39.52 |
| ATOM | 1381 N   | ALA | 179 | 30.869 | 41.550 | 39.171 | 1.00 16.72 |
| ATOM | 1382 CA  | ALA | 179 | 29.652 | 41.033 | 39.754 | 1.00 15.55 |
| ATOM | 1383 C   | ALA | 179 | 29.932 | 40.277 | 41.040 | 1.00 15.70 |
| ATOM | 1384 O   | ALA | 179 | 30.337 | 39.119 | 41.028 | 1.00 15.91 |
| ATOM | 1385 CB  | ALA | 179 | 28.853 | 40.197 | 38.731 | 1.00 14.08 |
| ATOM | 1386 N   | ASP | 180 | 29.694 | 40.946 | 42.155 | 1.00 8.88  |
| ATOM | 1387 CA  | ASP | 180 | 29.897 | 40.407 | 43.480 | 1.00 7.18  |
| ATOM | 1388 C   | ASP | 180 | 28.802 | 39.460 | 43.891 | 1.00 17.07 |
| ATOM | 1389 O   | ASP | 180 | 27.651 | 39.844 | 43.987 | 1.00 18.22 |



|      |          |     |     |        |        |        |            |
|------|----------|-----|-----|--------|--------|--------|------------|
| ATOM | 1390 CB  | ASP | 180 | 29.934 | 41.509 | 44.509 | 1.00 13.06 |
| ATOM | 1391 CG  | ASP | 180 | 31.285 | 41.902 | 44.935 | 1.00 46.28 |
| ATOM | 1392 OD1 | ASP | 180 | 31.981 | 41.206 | 45.655 | 1.00 60.46 |
| ATOM | 1393 OD2 | ASP | 180 | 31.574 | 43.121 | 44.560 | 1.00 46.61 |
| ATOM | 1394 N   | HIS | 181 | 29.173 | 38.242 | 44.197 | 1.00 14.51 |
| ATOM | 1395 CA  | HIS | 181 | 28.213 | 37.223 | 44.575 | 1.00 10.49 |
| ATOM | 1396 C   | HIS | 181 | 28.218 | 36.897 | 46.049 | 1.00 14.28 |
| ATOM | 1397 O   | HIS | 181 | 29.255 | 36.580 | 46.607 | 1.00 17.40 |
| ATOM | 1398 CB  | HIS | 181 | 28.450 | 35.915 | 43.769 | 1.00 9.89  |
| ATOM | 1399 CG  | HIS | 181 | 28.077 | 35.972 | 42.328 | 1.00 10.38 |
| ATOM | 1400 ND1 | HIS | 181 | 28.606 | 36.926 | 41.455 | 1.00 12.24 |
| ATOM | 1401 CD2 | HIS | 181 | 27.279 | 35.146 | 41.606 | 1.00 10.42 |
| ATOM | 1402 CE1 | HIS | 181 | 28.093 | 36.678 | 40.269 | 1.00 9.97  |
| ATOM | 1403 NE2 | HIS | 181 | 27.314 | 35.594 | 40.316 | 1.00 9.38  |
| ATOM | 1404 N   | TYR | 182 | 27.029 | 36.897 | 46.668 | 1.00 10.40 |
| ATOM | 1405 CA  | TYR | 182 | 26.848 | 36.518 | 48.062 | 1.00 13.86 |
| ATOM | 1406 C   | TYR | 182 | 25.871 | 35.393 | 48.089 | 1.00 20.61 |
| ATOM | 1407 O   | TYR | 182 | 24.819 | 35.520 | 47.532 | 1.00 16.35 |
| ATOM | 1408 CB  | TYR | 182 | 26.359 | 37.664 | 48.934 | 1.00 21.12 |
| ATOM | 1409 CG  | TYR | 182 | 27.421 | 38.693 | 49.062 | 1.00 34.16 |
| ATOM | 1410 CD1 | TYR | 182 | 27.521 | 39.715 | 48.120 | 1.00 46.06 |
| ATOM | 1411 CD2 | TYR | 182 | 28.389 | 38.616 | 50.064 | 1.00 38.56 |
| ATOM | 1412 CE1 | TYR | 182 | 28.532 | 40.674 | 48.197 | 1.00 57.53 |
| ATOM | 1413 CE2 | TYR | 182 | 29.418 | 39.559 | 50.147 | 1.00 40.76 |
| ATOM | 1414 CZ  | TYR | 182 | 29.480 | 40.594 | 49.216 | 1.00 54.61 |
| ATOM | 1415 OH  | TYR | 182 | 30.461 | 41.534 | 49.308 | 1.00 61.92 |
| ATOM | 1416 N   | GLN | 183 | 26.246 | 34.277 | 48.686 | 1.00 17.63 |
| ATOM | 1417 CA  | GLN | 183 | 25.410 | 33.104 | 48.583 | 1.00 16.37 |
| ATOM | 1418 C   | GLN | 183 | 25.289 | 32.311 | 49.863 | 1.00 21.39 |
| ATOM | 1419 O   | GLN | 183 | 26.260 | 32.174 | 50.623 | 1.00 19.86 |
| ATOM | 1420 CB  | GLN | 183 | 25.984 | 32.219 | 47.422 | 1.00 13.33 |
| ATOM | 1421 CG  | GLN | 183 | 25.651 | 30.688 | 47.457 | 1.00 17.38 |
| ATOM | 1422 CD  | GLN | 183 | 26.411 | 29.884 | 46.389 | 1.00 17.27 |
| ATOM | 1423 OE1 | GLN | 183 | 26.975 | 30.454 | 45.456 | 1.00 13.80 |
| ATOM | 1424 NE2 | GLN | 183 | 26.361 | 28.553 | 46.473 | 1.00 13.94 |
| ATOM | 1425 N   | GLN | 184 | 24.080 | 31.739 | 50.055 | 1.00 19.74 |
| ATOM | 1426 CA  | GLN | 184 | 23.760 | 30.829 | 51.168 | 1.00 16.55 |
| ATOM | 1427 C   | GLN | 184 | 23.033 | 29.582 | 50.658 | 1.00 13.60 |
| ATOM | 1428 O   | GLN | 184 | 22.219 | 29.640 | 49.747 | 1.00 18.01 |
| ATOM | 1429 CB  | GLN | 184 | 22.949 | 31.444 | 52.330 | 1.00 20.11 |
| ATOM | 1430 CG  | GLN | 184 | 23.364 | 32.855 | 52.768 | 1.00 74.84 |

**FIG. 5A1**



|      |      |     |     |     |        |        |        |      |        |
|------|------|-----|-----|-----|--------|--------|--------|------|--------|
| ATOM | 1472 | CB  | ASP | 190 | 15.195 | 16.734 | 58.955 | 1.00 | 63.89  |
| ATOM | 1473 | CG  | ASP | 190 | 14.592 | 15.365 | 58.686 | 1.00 | 99.67  |
| ATOM | 1474 | OD1 | ASP | 190 | 14.599 | 14.466 | 59.514 | 1.00 | 100.00 |
| ATOM | 1475 | OD2 | ASP | 190 | 14.088 | 15.240 | 57.470 | 1.00 | 100.00 |
| ATOM | 1476 | N   | GLY | 191 | 17.921 | 15.312 | 57.323 | 1.00 | 47.20  |
| ATOM | 1477 | CA  | GLY | 191 | 19.015 | 14.347 | 57.419 | 1.00 | 44.96  |
| ATOM | 1478 | C   | GLY | 191 | 20.359 | 15.044 | 57.587 | 1.00 | 34.43  |
| ATOM | 1479 | O   | GLY | 191 | 20.452 | 16.266 | 57.438 | 1.00 | 29.96  |
| ATOM | 1480 | N   | PRO | 192 | 21.402 | 14.264 | 57.905 | 1.00 | 27.26  |
| ATOM | 1481 | CA  | PRO | 192 | 22.737 | 14.834 | 58.100 | 1.00 | 24.01  |
| ATOM | 1482 | C   | PRO | 192 | 23.444 | 15.274 | 56.787 | 1.00 | 20.55  |
| ATOM | 1483 | O   | PRO | 192 | 23.323 | 14.648 | 55.740 | 1.00 | 23.84  |
| ATOM | 1484 | CB  | PRO | 192 | 23.583 | 13.764 | 58.825 | 1.00 | 21.00  |
| ATOM | 1485 | CG  | PRO | 192 | 22.739 | 12.501 | 58.915 | 1.00 | 27.49  |
| ATOM | 1486 | CD  | PRO | 192 | 21.330 | 12.863 | 58.448 | 1.00 | 27.26  |
| ATOM | 1487 | N   | VAL | 193 | 24.193 | 16.363 | 56.892 | 1.00 | 17.87  |
| ATOM | 1488 | CA  | VAL | 193 | 24.964 | 16.902 | 55.792 | 1.00 | 19.51  |
| ATOM | 1489 | C   | VAL | 193 | 26.380 | 17.108 | 56.249 | 1.00 | 22.37  |
| ATOM | 1490 | O   | VAL | 193 | 26.663 | 17.189 | 57.443 | 1.00 | 23.84  |
| ATOM | 1491 | CB  | VAL | 193 | 24.449 | 18.245 | 55.256 | 1.00 | 25.24  |
| ATOM | 1492 | CG1 | VAL | 193 | 23.059 | 18.118 | 54.632 | 1.00 | 21.90  |
| ATOM | 1493 | CG2 | VAL | 193 | 24.497 | 19.322 | 56.346 | 1.00 | 24.81  |
| ATOM | 1494 | N   | LEU | 194 | 27.253 | 17.241 | 55.277 | 1.00 | 19.04  |
| ATOM | 1495 | CA  | LEU | 194 | 28.654 | 17.438 | 55.516 | 1.00 | 20.29  |
| ATOM | 1496 | C   | LEU | 194 | 29.006 | 18.930 | 55.571 | 1.00 | 18.71  |
| ATOM | 1497 | O   | LEU | 194 | 28.907 | 19.615 | 54.591 | 1.00 | 20.13  |
| ATOM | 1498 | CB  | LEU | 194 | 29.412 | 16.806 | 54.327 | 1.00 | 22.92  |
| ATOM | 1499 | CG  | LEU | 194 | 29.994 | 15.423 | 54.542 | 1.00 | 30.60  |
| ATOM | 1500 | CD1 | LEU | 194 | 29.227 | 14.642 | 55.595 | 1.00 | 35.19  |
| ATOM | 1501 | CD2 | LEU | 194 | 30.048 | 14.672 | 53.211 | 1.00 | 25.61  |
| ATOM | 1502 | N   | LEU | 195 | 29.453 | 19.430 | 56.713 | 1.00 | 17.39  |
| ATOM | 1503 | CA  | LEU | 195 | 29.881 | 20.808 | 56.785 | 1.00 | 18.83  |
| ATOM | 1504 | C   | LEU | 195 | 31.389 | 20.837 | 56.579 | 1.00 | 28.32  |
| ATOM | 1505 | O   | LEU | 195 | 32.161 | 20.152 | 57.281 | 1.00 | 21.98  |
| ATOM | 1506 | CB  | LEU | 195 | 29.489 | 21.525 | 58.072 | 1.00 | 22.20  |
| ATOM | 1507 | CG  | LEU | 195 | 28.055 | 21.349 | 58.444 | 1.00 | 26.40  |
| ATOM | 1508 | CD1 | LEU | 195 | 27.937 | 21.508 | 59.941 | 1.00 | 31.99  |
| ATOM | 1509 | CD2 | LEU | 195 | 27.225 | 22.395 | 57.726 | 1.00 | 26.90  |
| ATOM | 1510 | N   | PRO | 196 | 31.789 | 21.610 | 55.597 | 1.00 | 21.58  |
| ATOM | 1511 | CA  | PRO | 196 | 33.177 | 21.666 | 55.154 | 1.00 | 22.17  |
| ATOM | 1512 | C   | PRO | 196 | 34.080 | 22.623 | 55.892 | 1.00 | 29.56  |

**FIG. 5AK**

|      |          |     |     |        |        |        |      |       |
|------|----------|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1513 O   | PRO | 196 | 33.635 | 23.588 | 56.490 | 1.00 | 29.04 |
| ATOM | 1514 CB  | PRO | 196 | 33.054 | 22.265 | 53.752 | 1.00 | 22.77 |
| ATOM | 1515 CG  | PRO | 196 | 31.761 | 23.104 | 53.735 | 1.00 | 18.99 |
| ATOM | 1516 CD  | PRO | 196 | 30.910 | 22.567 | 54.861 | 1.00 | 16.42 |
| ATOM | 1517 N   | ASP | 197 | 35.379 | 22.410 | 55.716 | 1.00 | 22.95 |
| ATOM | 1518 CA  | ASP | 197 | 36.364 | 23.370 | 56.134 | 1.00 | 19.71 |
| ATOM | 1519 C   | ASP | 197 | 36.556 | 24.295 | 54.931 | 1.00 | 24.74 |
| ATOM | 1520 O   | ASP | 197 | 36.251 | 23.913 | 53.800 | 1.00 | 24.88 |
| ATOM | 1521 CB  | ASP | 197 | 37.711 | 22.730 | 56.446 | 1.00 | 22.28 |
| ATOM | 1522 CG  | ASP | 197 | 37.690 | 21.913 | 57.687 | 1.00 | 43.93 |
| ATOM | 1523 OD1 | ASP | 197 | 36.912 | 22.117 | 58.608 | 1.00 | 53.47 |
| ATOM | 1524 OD2 | ASP | 197 | 38.634 | 21.006 | 57.694 | 1.00 | 31.58 |
| ATOM | 1525 N   | ASN | 198 | 37.062 | 25.501 | 55.168 | 1.00 | 19.74 |
| ATOM | 1526 CA  | ASN | 198 | 37.254 | 26.470 | 54.118 | 1.00 | 15.38 |
| ATOM | 1527 C   | ASN | 198 | 37.974 | 25.889 | 52.971 | 1.00 | 19.61 |
| ATOM | 1528 O   | ASN | 198 | 38.958 | 25.236 | 53.134 | 1.00 | 22.69 |
| ATOM | 1529 CB  | ASN | 198 | 38.013 | 27.704 | 54.614 | 1.00 | 24.48 |
| ATOM | 1530 CG  | ASN | 198 | 37.236 | 28.504 | 55.632 | 1.00 | 52.21 |
| ATOM | 1531 OD1 | ASN | 198 | 36.107 | 28.174 | 55.961 | 1.00 | 34.54 |
| ATOM | 1532 ND2 | ASN | 198 | 37.854 | 29.556 | 56.150 | 1.00 | 55.11 |
| ATOM | 1533 N   | HIS | 199 | 37.462 | 26.125 | 51.801 | 1.00 | 16.30 |
| ATOM | 1534 CA  | HIS | 199 | 38.071 | 25.627 | 50.616 | 1.00 | 15.80 |
| ATOM | 1535 C   | HIS | 199 | 37.496 | 26.357 | 49.450 | 1.00 | 14.85 |
| ATOM | 1536 O   | HIS | 199 | 36.757 | 27.295 | 49.643 | 1.00 | 16.45 |
| ATOM | 1537 CB  | HIS | 199 | 37.988 | 24.103 | 50.471 | 1.00 | 16.53 |
| ATOM | 1538 CG  | HIS | 199 | 36.597 | 23.628 | 50.218 | 1.00 | 16.65 |
| ATOM | 1539 ND1 | HIS | 199 | 35.695 | 23.491 | 51.244 | 1.00 | 17.85 |
| ATOM | 1540 CD2 | HIS | 199 | 35.987 | 23.282 | 49.048 | 1.00 | 18.67 |
| ATOM | 1541 CE1 | HIS | 199 | 34.561 | 23.052 | 50.688 | 1.00 | 19.45 |
| ATOM | 1542 NE2 | HIS | 199 | 34.716 | 22.905 | 49.364 | 1.00 | 18.74 |
| ATOM | 1543 N   | TYR | 200 | 37.879 | 25.998 | 48.247 | 1.00 | 12.56 |
| ATOM | 1544 CA  | TYR | 200 | 37.334 | 26.689 | 47.100 | 1.00 | 14.01 |
| ATOM | 1545 C   | TYR | 200 | 37.207 | 25.824 | 45.870 | 1.00 | 15.57 |
| ATOM | 1546 O   | TYR | 200 | 37.793 | 24.751 | 45.768 | 1.00 | 20.20 |
| ATOM | 1547 CB  | TYR | 200 | 38.030 | 28.011 | 46.779 | 1.00 | 19.79 |
| ATOM | 1548 CG  | TYR | 200 | 39.382 | 27.745 | 46.202 | 1.00 | 22.25 |
| ATOM | 1549 CD1 | TYR | 200 | 39.543 | 27.526 | 44.835 | 1.00 | 22.53 |
| ATOM | 1550 CD2 | TYR | 200 | 40.473 | 27.605 | 47.057 | 1.00 | 25.73 |
| ATOM | 1551 CE1 | TYR | 200 | 40.800 | 27.222 | 44.317 | 1.00 | 35.51 |
| ATOM | 1552 CE2 | TYR | 200 | 41.739 | 27.314 | 46.559 | 1.00 | 29.34 |
| ATOM | 1553 CZ  | TYR | 200 | 41.896 | 27.132 | 45.186 | 1.00 | 54.14 |

**FIG. 5AL**

|      |          |     |     |        |        |        |      |       |
|------|----------|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1554 OH  | TYR | 200 | 43.153 | 26.820 | 44.703 | 1.00 | 62.66 |
| ATOM | 1555 N   | LEU | 201 | 36.393 | 26.309 | 44.946 | 1.00 | 15.07 |
| ATOM | 1556 CA  | LEU | 201 | 36.147 | 25.680 | 43.678 | 1.00 | 11.01 |
| ATOM | 1557 C   | LEU | 201 | 36.753 | 26.532 | 42.593 | 1.00 | 17.30 |
| ATOM | 1558 O   | LEU | 201 | 36.619 | 27.753 | 42.610 | 1.00 | 20.19 |
| ATOM | 1559 CB  | LEU | 201 | 34.628 | 25.518 | 43.354 | 1.00 | 10.09 |
| ATOM | 1560 CG  | LEU | 201 | 33.749 | 25.027 | 44.480 | 1.00 | 13.41 |
| ATOM | 1561 CD1 | LEU | 201 | 32.293 | 24.938 | 43.954 | 1.00 | 17.11 |
| ATOM | 1562 CD2 | LEU | 201 | 34.196 | 23.635 | 44.927 | 1.00 | 23.03 |
| ATOM | 1563 N   | SER | 202 | 37.407 | 25.868 | 41.651 | 1.00 | 10.75 |
| ATOM | 1564 CA  | SER | 202 | 38.047 | 26.490 | 40.528 | 1.00 | 8.51  |
| ATOM | 1565 C   | SER | 202 | 37.222 | 26.189 | 39.294 | 1.00 | 11.56 |
| ATOM | 1566 O   | SER | 202 | 36.919 | 25.038 | 38.996 | 1.00 | 14.58 |
| ATOM | 1567 CB  | SER | 202 | 39.485 | 25.987 | 40.442 | 1.00 | 15.68 |
| ATOM | 1568 OG  | SER | 202 | 40.067 | 26.353 | 39.228 | 1.00 | 36.44 |
| ATOM | 1569 N   | THR | 203 | 36.798 | 27.241 | 38.601 | 1.00 | 12.36 |
| ATOM | 1570 CA  | THR | 203 | 35.879 | 27.067 | 37.499 | 1.00 | 15.60 |
| ATOM | 1571 C   | THR | 203 | 36.417 | 27.521 | 36.195 | 1.00 | 20.19 |
| ATOM | 1572 O   | THR | 203 | 37.192 | 28.472 | 36.114 | 1.00 | 18.29 |
| ATOM | 1573 CB  | THR | 203 | 34.565 | 27.892 | 37.757 | 1.00 | 20.51 |
| ATOM | 1574 OG1 | THR | 203 | 34.911 | 29.260 | 37.780 | 1.00 | 20.39 |
| ATOM | 1575 CG2 | THR | 203 | 33.935 | 27.557 | 39.093 | 1.00 | 6.80  |
| ATOM | 1576 N   | GLN | 204 | 35.913 | 26.883 | 35.164 | 1.00 | 10.30 |
| ATOM | 1577 CA  | GLN | 204 | 36.173 | 27.271 | 33.807 | 1.00 | 14.85 |
| ATOM | 1578 C   | GLN | 204 | 34.956 | 26.980 | 32.921 | 1.00 | 23.14 |
| ATOM | 1579 O   | GLN | 204 | 34.334 | 25.932 | 33.056 | 1.00 | 21.66 |
| ATOM | 1580 CB  | GLN | 204 | 37.475 | 26.696 | 33.237 | 1.00 | 20.33 |
| ATOM | 1581 CG  | GLN | 204 | 37.271 | 25.371 | 32.518 | 1.00 | 40.16 |
| ATOM | 1582 CD  | GLN | 204 | 38.588 | 24.722 | 32.193 | 1.00 | 59.76 |
| ATOM | 1583 OE1 | GLN | 204 | 39.011 | 24.716 | 31.035 | 1.00 | 41.80 |
| ATOM | 1584 NE2 | GLN | 204 | 39.276 | 24.241 | 33.235 | 1.00 | 34.80 |
| ATOM | 1585 N   | SER | 205 | 34.619 | 27.913 | 32.021 | 1.00 | 15.83 |
| ATOM | 1586 CA  | SER | 205 | 33.447 | 27.762 | 31.172 | 1.00 | 14.60 |
| ATOM | 1587 C   | SER | 205 | 33.654 | 28.307 | 29.783 | 1.00 | 20.21 |
| ATOM | 1588 O   | SER | 205 | 34.282 | 29.337 | 29.581 | 1.00 | 17.82 |
| ATOM | 1589 CB  | SER | 205 | 32.197 | 28.445 | 31.758 | 1.00 | 11.88 |
| ATOM | 1590 OG  | SER | 205 | 32.121 | 28.406 | 33.177 | 1.00 | 15.45 |
| ATOM | 1591 N   | ALA | 206 | 33.065 | 27.630 | 28.827 | 1.00 | 13.00 |
| ATOM | 1592 CA  | ALA | 206 | 33.079 | 28.029 | 27.426 | 1.00 | 9.99  |
| ATOM | 1593 C   | ALA | 206 | 31.623 | 28.192 | 26.924 | 1.00 | 21.23 |
| ATOM | 1594 O   | ALA | 206 | 30.809 | 27.306 | 27.139 | 1.00 | 14.10 |

**FIG. 5AM**



|      |          |     |     |        |        |        |            |
|------|----------|-----|-----|--------|--------|--------|------------|
| ATOM | 1636 C   | ASN | 212 | 19.642 | 25.894 | 14.497 | 1.00 41.92 |
| ATOM | 1637 O   | ASN | 212 | 18.485 | 25.518 | 14.263 | 1.00 42.30 |
| ATOM | 1638 CB  | ASN | 212 | 20.788 | 24.028 | 13.236 | 1.00 48.64 |
| ATOM | 1639 CG  | ASN | 212 | 21.883 | 23.678 | 12.230 | 1.00 53.61 |
| ATOM | 1640 N   | GLU | 213 | 19.947 | 26.675 | 15.520 | 1.00 27.84 |
| ATOM | 1641 CA  | GLU | 213 | 18.953 | 27.080 | 16.478 | 1.00 20.43 |
| ATOM | 1642 C   | GLU | 213 | 18.485 | 28.527 | 16.241 | 1.00 29.95 |
| ATOM | 1643 O   | GLU | 213 | 19.247 | 29.475 | 16.324 | 1.00 32.77 |
| ATOM | 1644 CB  | GLU | 213 | 19.535 | 26.878 | 17.894 | 1.00 16.45 |
| ATOM | 1645 CG  | GLU | 213 | 18.594 | 27.326 | 18.995 | 1.00 18.29 |
| ATOM | 1646 CD  | GLU | 213 | 17.229 | 26.703 | 18.853 | 1.00 38.01 |
| ATOM | 1647 OE1 | GLU | 213 | 16.238 | 27.334 | 18.508 | 1.00 25.07 |
| ATOM | 1648 OE2 | GLU | 213 | 17.223 | 25.423 | 19.122 | 1.00 19.17 |
| ATOM | 1649 N   | LYS | 214 | 17.223 | 28.713 | 15.963 | 1.00 22.99 |
| ATOM | 1650 CA  | LYS | 214 | 16.721 | 30.081 | 15.726 | 1.00 22.84 |
| ATOM | 1651 C   | LYS | 214 | 16.252 | 30.778 | 16.982 | 1.00 21.50 |
| ATOM | 1652 O   | LYS | 214 | 16.130 | 32.016 | 17.032 | 1.00 28.15 |
| ATOM | 1653 CB  | LYS | 214 | 15.653 | 30.197 | 14.606 | 1.00 27.58 |
| ATOM | 1654 CG  | LYS | 214 | 16.153 | 29.816 | 13.209 | 1.00 32.71 |
| ATOM | 1655 CD  | LYS | 214 | 16.752 | 30.979 | 12.431 | 1.00 55.31 |
| ATOM | 1656 N   | ARG | 215 | 15.947 | 30.028 | 18.014 | 1.00 14.52 |
| ATOM | 1657 CA  | ARG | 215 | 15.518 | 30.726 | 19.209 | 1.00 15.58 |
| ATOM | 1658 C   | ARG | 215 | 16.719 | 31.382 | 19.892 | 1.00 21.87 |
| ATOM | 1659 O   | ARG | 215 | 17.848 | 31.075 | 19.572 | 1.00 26.69 |
| ATOM | 1660 CB  | ARG | 215 | 14.808 | 29.804 | 20.159 | 1.00 18.82 |
| ATOM | 1661 CG  | ARG | 215 | 13.660 | 29.067 | 19.475 | 1.00 23.30 |
| ATOM | 1662 CD  | ARG | 215 | 13.220 | 27.806 | 20.205 | 1.00 15.45 |
| ATOM | 1663 NE  | ARG | 215 | 14.107 | 26.668 | 19.929 | 1.00 28.08 |
| ATOM | 1664 CZ  | ARG | 215 | 14.022 | 25.473 | 20.543 | 1.00 21.38 |
| ATOM | 1665 NH1 | ARG | 215 | 13.074 | 25.215 | 21.455 | 1.00 23.92 |
| ATOM | 1666 NH2 | ARG | 215 | 14.893 | 24.514 | 20.225 | 1.00 20.46 |
| ATOM | 1667 N   | ASP | 216 | 16.466 | 32.275 | 20.830 | 1.00 16.72 |
| ATOM | 1668 CA  | ASP | 216 | 17.556 | 32.895 | 21.617 | 1.00 19.06 |
| ATOM | 1669 C   | ASP | 216 | 18.047 | 31.817 | 22.607 | 1.00 20.02 |
| ATOM | 1670 O   | ASP | 216 | 17.261 | 31.214 | 23.350 | 1.00 18.45 |
| ATOM | 1671 CB  | ASP | 216 | 17.066 | 34.169 | 22.383 | 1.00 21.33 |
| ATOM | 1672 CG  | ASP | 216 | 18.138 | 35.140 | 22.893 | 1.00 20.97 |
| ATOM | 1673 OD1 | ASP | 216 | 17.869 | 36.079 | 23.620 | 1.00 28.46 |
| ATOM | 1674 OD2 | ASP | 216 | 19.342 | 34.900 | 22.441 | 1.00 20.37 |
| ATOM | 1675 N   | HIS | 217 | 19.332 | 31.537 | 22.589 | 1.00 13.18 |
| ATOM | 1676 CA  | HIS | 217 | 19.813 | 30.482 | 23.433 | 1.00 11.21 |

**FIG. 5A0**

|      |          |     |     |        |        |        |            |
|------|----------|-----|-----|--------|--------|--------|------------|
| ATOM | 1677 C   | HIS | 217 | 21.313 | 30.614 | 23.723 | 1.00 21.35 |
| ATOM | 1678 O   | HIS | 217 | 22.014 | 31.471 | 23.163 | 1.00 15.03 |
| ATOM | 1679 CB  | HIS | 217 | 19.587 | 29.168 | 22.690 | 1.00 13.03 |
| ATOM | 1680 CG  | HIS | 217 | 20.525 | 29.025 | 21.542 | 1.00 15.49 |
| ATOM | 1681 ND1 | HIS | 217 | 20.463 | 29.871 | 20.449 | 1.00 17.88 |
| ATOM | 1682 CD2 | HIS | 217 | 21.589 | 28.172 | 21.361 | 1.00 17.51 |
| ATOM | 1683 CE1 | HIS | 217 | 21.457 | 29.524 | 19.635 | 1.00 17.94 |
| ATOM | 1684 NE2 | HIS | 217 | 22.152 | 28.501 | 20.151 | 1.00 17.59 |
| ATOM | 1685 N   | MSE | 218 | 21.794 | 29.725 | 24.576 | 1.00 11.26 |
| ATOM | 1686 CA  | MSE | 218 | 23.186 | 29.642 | 24.887 | 1.00 11.49 |
| ATOM | 1687 C   | MSE | 218 | 23.560 | 28.198 | 25.094 | 1.00 24.15 |
| ATOM | 1688 O   | MSE | 218 | 22.822 | 27.446 | 25.751 | 1.00 20.70 |
| ATOM | 1689 CB  | MSE | 218 | 23.539 | 30.421 | 26.172 | 1.00 12.84 |
| ATOM | 1690 CG  | MSE | 218 | 24.809 | 30.004 | 26.907 | 1.00 12.59 |
| ATOM | 1691 SE  | MSE | 218 | 25.267 | 31.128 | 28.434 | 1.00 29.94 |
| ATOM | 1692 CE  | MSE | 218 | 24.039 | 30.502 | 29.781 | 1.00 13.54 |
| ATOM | 1693 N   | VAL | 219 | 24.727 | 27.824 | 24.558 | 1.00 15.62 |
| ATOM | 1694 CA  | VAL | 219 | 25.309 | 26.518 | 24.782 | 1.00 10.58 |
| ATOM | 1695 C   | VAL | 219 | 26.473 | 26.689 | 25.753 | 1.00 16.54 |
| ATOM | 1696 O   | VAL | 219 | 27.280 | 27.604 | 25.585 | 1.00 15.54 |
| ATOM | 1697 CB  | VAL | 219 | 25.774 | 25.883 | 23.498 | 1.00 15.08 |
| ATOM | 1698 CG1 | VAL | 219 | 26.330 | 24.495 | 23.824 | 1.00 14.34 |
| ATOM | 1699 CG2 | VAL | 219 | 24.599 | 25.766 | 22.512 | 1.00 15.78 |
| ATOM | 1700 N   | LEU | 220 | 26.523 | 25.836 | 26.783 | 1.00 10.95 |
| ATOM | 1701 CA  | LEU | 220 | 27.490 | 25.939 | 27.850 | 1.00 11.01 |
| ATOM | 1702 C   | LEU | 220 | 28.206 | 24.643 | 28.184 | 1.00 21.26 |
| ATOM | 1703 O   | LEU | 220 | 27.592 | 23.577 | 28.324 | 1.00 15.94 |
| ATOM | 1704 CB  | LEU | 220 | 26.807 | 26.545 | 29.100 | 1.00 13.75 |
| ATOM | 1705 CG  | LEU | 220 | 27.624 | 26.578 | 30.402 | 1.00 21.10 |
| ATOM | 1706 CD1 | LEU | 220 | 28.433 | 27.875 | 30.483 | 1.00 23.53 |
| ATOM | 1707 CD2 | LEU | 220 | 26.663 | 26.556 | 31.586 | 1.00 22.04 |
| ATOM | 1708 N   | LEU | 221 | 29.570 | 24.758 | 28.273 | 1.00 19.04 |
| ATOM | 1709 CA  | LEU | 221 | 30.498 | 23.666 | 28.697 | 1.00 13.22 |
| ATOM | 1710 C   | LEU | 221 | 31.309 | 24.178 | 29.887 | 1.00 10.73 |
| ATOM | 1711 O   | LEU | 221 | 31.846 | 25.267 | 29.857 | 1.00 12.98 |
| ATOM | 1712 CB  | LEU | 221 | 31.382 | 23.102 | 27.549 | 1.00 13.74 |
| ATOM | 1713 CG  | LEU | 221 | 32.580 | 22.257 | 28.045 | 1.00 18.64 |
| ATOM | 1714 CD1 | LEU | 221 | 32.149 | 20.868 | 28.496 | 1.00 17.38 |
| ATOM | 1715 CD2 | LEU | 221 | 33.571 | 22.109 | 26.911 | 1.00 26.97 |
| ATOM | 1716 N   | GLU | 222 | 31.316 | 23.446 | 30.963 | 1.00 9.31  |
| ATOM | 1717 CA  | GLU | 222 | 31.936 | 23.929 | 32.144 | 1.00 9.97  |

**FIG. 5AP**



|      |          |     |     |        |        |        |            |
|------|----------|-----|-----|--------|--------|--------|------------|
| ATOM | 1718 C   | GLU | 222 | 32.548 | 22.803 | 32.951 | 1.00 12.94 |
| ATOM | 1719 O   | GLU | 222 | 32.072 | 21.662 | 32.966 | 1.00 13.38 |
| ATOM | 1720 CB  | GLU | 222 | 30.836 | 24.762 | 32.896 | 1.00 12.14 |
| ATOM | 1721 CG  | GLU | 222 | 31.092 | 25.119 | 34.364 | 1.00 13.88 |
| ATOM | 1722 CD  | GLU | 222 | 29.895 | 25.891 | 34.934 | 1.00 13.57 |
| ATOM | 1723 OE1 | GLU | 222 | 29.128 | 26.477 | 34.240 | 1.00 19.47 |
| ATOM | 1724 OE2 | GLU | 222 | 29.752 | 25.789 | 36.207 | 1.00 18.51 |
| ATOM | 1725 N   | PHE | 223 | 33.687 | 23.123 | 33.542 | 1.00 15.86 |
| ATOM | 1726 CA  | PHE | 223 | 34.476 | 22.227 | 34.373 | 1.00 9.34  |
| ATOM | 1727 C   | PHE | 223 | 34.711 | 22.864 | 35.722 | 1.00 11.08 |
| ATOM | 1728 O   | PHE | 223 | 35.028 | 24.055 | 35.828 | 1.00 19.86 |
| ATOM | 1729 CB  | PHE | 223 | 35.847 | 21.919 | 33.684 | 1.00 8.30  |
| ATOM | 1730 CG  | PHE | 223 | 35.703 | 21.134 | 32.431 | 1.00 10.50 |
| ATOM | 1731 CD1 | PHE | 223 | 35.570 | 19.747 | 32.469 | 1.00 13.56 |
| ATOM | 1732 CD2 | PHE | 223 | 35.750 | 21.750 | 31.184 | 1.00 11.32 |
| ATOM | 1733 CE1 | PHE | 223 | 35.481 | 19.010 | 31.287 | 1.00 12.58 |
| ATOM | 1734 CE2 | PHE | 223 | 35.667 | 21.032 | 29.995 | 1.00 12.17 |
| ATOM | 1735 CZ  | PHE | 223 | 35.521 | 19.648 | 30.050 | 1.00 10.87 |
| ATOM | 1736 N   | VAL | 224 | 34.542 | 22.081 | 36.765 | 1.00 9.28  |
| ATOM | 1737 CA  | VAL | 224 | 34.708 | 22.587 | 38.080 | 1.00 11.18 |
| ATOM | 1738 C   | VAL | 224 | 35.324 | 21.553 | 39.010 | 1.00 17.52 |
| ATOM | 1739 O   | VAL | 224 | 34.848 | 20.418 | 39.137 | 1.00 13.17 |
| ATOM | 1740 CB  | VAL | 224 | 33.370 | 23.078 | 38.662 | 1.00 16.61 |
| ATOM | 1741 CG1 | VAL | 224 | 33.622 | 23.736 | 40.022 | 1.00 13.90 |
| ATOM | 1742 CG2 | VAL | 224 | 32.674 | 24.048 | 37.697 | 1.00 13.85 |
| ATOM | 1743 N   | THR | 225 | 36.380 | 21.965 | 39.676 | 1.00 11.71 |
| ATOM | 1744 CA  | THR | 225 | 37.026 | 21.099 | 40.617 | 1.00 11.61 |
| ATOM | 1745 C   | THR | 225 | 37.366 | 21.798 | 41.927 | 1.00 14.76 |
| ATOM | 1746 O   | THR | 225 | 37.702 | 23.002 | 41.962 | 1.00 16.64 |
| ATOM | 1747 CB  | THR | 225 | 38.162 | 20.279 | 40.014 | 1.00 20.38 |
| ATOM | 1748 OG1 | THR | 225 | 39.288 | 20.337 | 40.822 | 1.00 30.44 |
| ATOM | 1749 CG2 | THR | 225 | 38.468 | 20.722 | 38.631 | 1.00 10.89 |
| ATOM | 1750 N   | ALA | 226 | 37.222 | 21.065 | 43.011 | 1.00 7.89  |
| ATOM | 1751 CA  | ALA | 226 | 37.478 | 21.595 | 44.352 | 1.00 11.63 |
| ATOM | 1752 C   | ALA | 226 | 38.969 | 21.558 | 44.677 | 1.00 16.61 |
| ATOM | 1753 O   | ALA | 226 | 39.687 | 20.699 | 44.199 | 1.00 15.60 |
| ATOM | 1754 CB  | ALA | 226 | 36.695 | 20.847 | 45.444 | 1.00 12.17 |
| ATOM | 1755 N   | ALA | 227 | 39.395 | 22.490 | 45.479 | 1.00 13.95 |
| ATOM | 1756 CA  | ALA | 227 | 40.789 | 22.550 | 45.871 | 1.00 19.64 |
| ATOM | 1757 C   | ALA | 227 | 40.987 | 23.299 | 47.170 | 1.00 26.33 |
| ATOM | 1758 O   | ALA | 227 | 40.042 | 23.715 | 47.840 | 1.00 25.39 |

**FIG. 5AQ**

|      |      |     |     |     |        |        |        |      |       |
|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1759 | CB  | ALA | 227 | 41.557 | 23.246 | 44.760 | 1.00 | 18.42 |
| ATOM | 1760 | N   | GLY | 228 | 42.245 | 23.476 | 47.523 | 1.00 | 23.28 |
| ATOM | 1761 | CA  | GLY | 228 | 42.616 | 24.292 | 48.658 | 1.00 | 21.61 |
| ATOM | 1762 | C   | GLY | 228 | 42.805 | 23.562 | 49.939 | 1.00 | 32.93 |
| ATOM | 1763 | O   | GLY | 228 | 42.948 | 24.201 | 51.009 | 1.00 | 32.53 |
| ATOM | 1764 | N   | ILE | 229 | 42.803 | 22.231 | 49.842 | 1.00 | 33.59 |
| ATOM | 1765 | CA  | ILE | 229 | 43.006 | 21.375 | 50.998 | 1.00 | 31.81 |
| ATOM | 1766 | C   | ILE | 229 | 44.016 | 20.291 | 50.633 | 1.00 | 28.78 |
| ATOM | 1767 | O   | ILE | 229 | 45.090 | 20.176 | 51.246 | 1.00 | 96.02 |
| ATOM | 1768 | CB  | ILE | 229 | 41.691 | 20.772 | 51.519 | 1.00 | 35.70 |
| ATOM | 1769 | CG1 | ILE | 229 | 40.890 | 21.807 | 52.325 | 1.00 | 30.66 |
| ATOM | 1770 | CG2 | ILE | 229 | 41.990 | 19.549 | 52.392 | 1.00 | 33.37 |
| ATOM | 1771 | CD1 | ILE | 229 | 39.386 | 21.715 | 52.092 | 1.00 | 38.74 |
| ATOM | 1772 | O   | HOH | 301 | 27.530 | 12.735 | 38.010 | 1.00 | 15.09 |
| ATOM | 1773 | O   | HOH | 302 | 23.919 | 34.589 | 37.331 | 1.00 | 10.29 |
| ATOM | 1774 | O   | HOH | 303 | 27.229 | 34.816 | 35.487 | 1.00 | 11.12 |
| ATOM | 1775 | O   | HOH | 304 | 29.914 | 18.943 | 44.692 | 1.00 | 16.10 |
| ATOM | 1776 | O   | HOH | 305 | 30.956 | 21.886 | 49.900 | 1.00 | 21.47 |
| ATOM | 1777 | O   | HOH | 306 | 20.072 | 31.196 | 43.592 | 1.00 | 16.85 |
| ATOM | 1778 | O   | HOH | 307 | 26.660 | 48.630 | 33.797 | 1.00 | 24.67 |
| ATOM | 1779 | O   | HOH | 308 | 22.329 | 33.239 | 41.399 | 1.00 | 14.11 |
| ATOM | 1780 | O   | HOH | 309 | 22.465 | 48.025 | 32.810 | 1.00 | 18.51 |
| ATOM | 1781 | O   | HOH | 310 | 31.012 | 39.126 | 29.118 | 1.00 | 16.01 |
| ATOM | 1782 | O   | HOH | 311 | 33.067 | 35.809 | 33.010 | 1.00 | 19.92 |
| ATOM | 1783 | O   | HOH | 312 | 31.130 | 37.076 | 30.841 | 1.00 | 12.68 |
| ATOM | 1784 | O   | HOH | 313 | 40.304 | 30.058 | 38.616 | 1.00 | 56.07 |
| ATOM | 1785 | O   | HOH | 314 | 34.166 | 26.379 | 57.222 | 1.00 | 22.58 |
| ATOM | 1786 | O   | HOH | 315 | 36.215 | 35.320 | 43.598 | 1.00 | 22.30 |
| ATOM | 1787 | O   | HOH | 316 | 33.866 | 29.786 | 34.671 | 1.00 | 12.21 |
| ATOM | 1865 | O   | HOH | 317 | 42.341 | 20.166 | 43.534 | 1.00 | 26.67 |
| ATOM | 1788 | O   | HOH | 318 | 10.270 | 28.684 | 30.403 | 1.00 | 43.66 |
| ATOM | 1789 | O   | HOH | 319 | 28.448 | 16.822 | 30.655 | 1.00 | 25.44 |
| ATOM | 1790 | O   | HOH | 320 | 30.612 | 20.922 | 37.231 | 1.00 | 21.57 |
| ATOM | 1791 | O   | HOH | 321 | 11.639 | 37.421 | 26.801 | 1.00 | 34.12 |
| ATOM | 1792 | O   | HOH | 322 | 27.030 | 37.308 | 36.869 | 1.00 | 13.10 |
| ATOM | 1793 | O   | HOH | 323 | 33.119 | 14.524 | 43.070 | 1.00 | 30.93 |
| ATOM | 1794 | O   | HOH | 324 | 37.973 | 14.036 | 53.352 | 1.00 | 35.39 |
| ATOM | 1795 | O   | HOH | 235 | 32.015 | 49.100 | 37.028 | 1.00 | 59.37 |
| ATOM | 1796 | O   | HOH | 326 | 11.959 | 12.020 | 43.429 | 1.00 | 29.06 |
| ATOM | 1797 | O   | HOH | 327 | 36.760 | 29.941 | 31.666 | 1.00 | 22.03 |
| ATOM | 1864 | O   | HOH | 328 | 15.305 | 26.513 | 15.694 | 1.00 | 39.62 |

**FIG. 5AR**

|      |        |     |     |        |        |        |            |
|------|--------|-----|-----|--------|--------|--------|------------|
| ATOM | 1798 O | HOH | 329 | 33.005 | 46.924 | 36.994 | 1.00 22.07 |
| ATOM | 1863 O | HOH | 330 | 23.801 | 36.134 | 22.715 | 1.00 45.30 |
| ATOM | 1799 O | HOH | 331 | 33.609 | 31.296 | 26.261 | 1.00 23.65 |
| ATOM | 1862 O | HOH | 332 | 34.942 | 24.780 | 29.532 | 1.00 38.93 |
| ATOM | 1800 O | HOH | 333 | 25.235 | 12.919 | 54.611 | 1.00 36.20 |
| ATOM | 1861 O | HOH | 334 | 38.048 | 23.467 | 36.645 | 1.00 37.73 |
| ATOM | 1801 O | HOH | 335 | 12.284 | 43.511 | 38.338 | 1.00 33.79 |
| ATOM | 1802 O | HOH | 336 | 9.826  | 47.020 | 32.568 | 1.00 46.67 |
| ATOM | 1803 O | HOH | 337 | 7.671  | 41.532 | 29.806 | 1.00 40.88 |
| ATOM | 1804 O | HOH | 338 | 15.430 | 23.713 | 26.808 | 1.00 34.73 |
| ATOM | 1805 O | HOH | 339 | 24.344 | 20.385 | 25.121 | 1.00 53.42 |
| ATOM | 1806 O | HOH | 340 | 31.550 | 10.656 | 40.819 | 1.00 47.85 |
| ATOM | 1807 O | HOH | 341 | 17.569 | 23.030 | 25.796 | 1.00 28.17 |
| ATOM | 1808 O | HOH | 342 | 19.174 | 38.552 | 23.965 | 1.00 45.54 |
| ATOM | 1809 O | HOH | 343 | 24.268 | 37.527 | 25.415 | 1.00 30.97 |
| ATOM | 1810 O | HOH | 344 | 21.266 | 29.482 | 41.551 | 1.00 19.69 |
| ATOM | 1811 O | HOH | 345 | 20.668 | 26.999 | 41.933 | 1.00 11.81 |
| ATOM | 1812 O | HOH | 346 | 24.780 | 24.795 | 43.460 | 1.00 20.95 |
| ATOM | 1813 O | HOH | 347 | 42.962 | 13.170 | 46.312 | 1.00 31.00 |
| ATOM | 1814 O | HOH | 348 | 32.322 | 14.088 | 47.013 | 1.00 28.20 |
| ATOM | 1815 O | HOH | 349 | 31.708 | 13.186 | 49.679 | 1.00 35.57 |
| ATOM | 1816 O | HOH | 350 | 22.408 | 35.801 | 50.514 | 1.00 40.71 |
| ATOM | 1817 O | HOH | 351 | 25.366 | 47.090 | 42.583 | 1.00 38.15 |
| ATOM | 1818 O | HOH | 352 | 27.243 | 47.647 | 43.977 | 1.00 41.55 |
| ATOM | 1819 O | HOH | 353 | 29.868 | 45.076 | 42.906 | 1.00 29.32 |
| ATOM | 1820 O | HOH | 354 | 14.175 | 22.269 | 42.680 | 1.00 74.11 |
| ATOM | 1821 O | HOH | 355 | 13.414 | 10.739 | 35.791 | 1.00 29.92 |
| ATOM | 1822 O | HOH | 356 | 20.338 | 9.974  | 37.765 | 1.00 30.46 |
| ATOM | 1823 O | HOH | 357 | 23.520 | 40.420 | 24.953 | 1.00 29.75 |
| ATOM | 1824 O | HOH | 358 | 25.718 | 41.692 | 26.023 | 1.00 30.43 |
| ATOM | 1825 O | HOH | 359 | 26.826 | 38.466 | 25.345 | 1.00 31.72 |
| ATOM | 1826 O | HOH | 360 | 37.768 | 42.373 | 25.123 | 1.00 41.53 |
| ATOM | 1827 O | HOH | 361 | 40.078 | 42.268 | 25.852 | 1.00 37.12 |
| ATOM | 1828 O | HOH | 362 | 31.483 | 38.677 | 22.083 | 1.00 54.21 |
| ATOM | 1829 O | HOH | 363 | 33.891 | 37.723 | 30.126 | 1.00 23.35 |
| ATOM | 1860 O | HOH | 364 | 39.936 | 26.543 | 36.329 | 1.00 47.93 |
| ATOM | 1830 O | HOH | 365 | 36.631 | 34.210 | 41.636 | 1.00 62.74 |
| ATOM | 1831 O | HOH | 366 | 37.038 | 29.783 | 52.197 | 1.00 40.07 |
| ATOM | 1832 O | HOH | 367 | 37.289 | 37.407 | 40.231 | 1.00 37.59 |
| ATOM | 1833 O | HOH | 368 | 18.930 | 17.517 | 52.472 | 1.00 35.80 |
| ATOM | 1834 O | HOH | 369 | 19.506 | 18.914 | 57.913 | 1.00 45.72 |

FIG. 5AS

|      |        |     |     |        |        |        |      |       |
|------|--------|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1835 O | HOH | 370 | 30.903 | 26.708 | 41.139 | 1.00 | 21.54 |
| ATOM | 1836 O | HOH | 371 | 30.369 | 25.678 | 24.583 | 1.00 | 22.46 |
| ATOM | 1837 O | HOH | 372 | 21.000 | 33.705 | 20.826 | 1.00 | 26.00 |
| ATOM | 1838 O | HOH | 373 | 13.648 | 32.794 | 21.329 | 1.00 | 27.98 |
| ATOM | 1839 O | HOH | 374 | 29.735 | 25.683 | 38.707 | 1.00 | 21.00 |
| ATOM | 1859 O | HOH | 375 | 33.670 | 24.419 | 60.503 | 1.00 | 50.04 |
| ATOM | 1840 O | HOH | 376 | 30.034 | 11.047 | 37.420 | 1.00 | 43.28 |
| ATOM | 1841 O | HOH | 377 | 8.662  | 35.846 | 35.068 | 1.00 | 51.94 |
| ATOM | 1842 O | HOH | 378 | 10.847 | 36.466 | 39.503 | 1.00 | 42.32 |
| ATOM | 1843 O | HOH | 379 | 14.395 | 48.943 | 39.085 | 1.00 | 29.72 |
| ATOM | 1844 O | HOH | 380 | 36.676 | 11.660 | 40.172 | 1.00 | 39.81 |
| ATOM | 1845 O | HOH | 381 | 35.968 | 7.212  | 34.763 | 1.00 | 58.66 |
| ATOM | 1846 O | HOH | 382 | 17.426 | 21.988 | 21.077 | 1.00 | 41.69 |
| ATOM | 1847 O | HOH | 383 | 29.837 | 22.623 | 39.378 | 1.00 | 32.82 |
| ATOM | 1848 O | HOH | 384 | 23.855 | 29.386 | 55.164 | 1.00 | 55.00 |
| ATOM | 1849 O | HOH | 385 | 17.408 | 35.360 | 47.495 | 1.00 | 61.61 |
| ATOM | 1850 O | HOH | 386 | 27.900 | 49.720 | 42.445 | 1.00 | 47.70 |
| ATOM | 1851 O | HOH | 387 | 13.932 | 36.230 | 44.385 | 1.00 | 45.08 |
| ATOM | 1852 O | HOH | 388 | 12.650 | 28.021 | 43.288 | 1.00 | 49.86 |
| ATOM | 1853 O | HOH | 389 | 16.974 | 42.367 | 43.435 | 1.00 | 34.38 |
| ATOM | 1854 O | HOH | 390 | 37.335 | 42.653 | 28.295 | 1.00 | 64.46 |
| ATOM | 1855 O | HOH | 391 | 29.701 | 49.856 | 35.323 | 1.00 | 62.61 |
| ATOM | 1856 O | HOH | 392 | 27.267 | 50.835 | 33.976 | 1.00 | 66.60 |
| ATOM | 1857 O | HOH | 393 | 19.661 | 29.181 | 51.537 | 1.00 | 34.01 |
| ATOM | 1858 O | HOH | 394 | 29.412 | 17.505 | 59.089 | 1.00 | 51.78 |
| TER  |        |     |     |        |        |        |      |       |
| END  |        |     |     |        |        |        |      |       |

**FIG. 5AT**

